2,6,10-Trimethyltridecane

Inchi: InChI=1S/C16H34/c1-6-9-15(4)12-8-13-16(5)11-7-10-14(2)3/h14-16H,6-13H2,1-5H3
InchiKey: MSRQAOLBRXEIHE-UHFFFAOYSA-N
Formula: C16H34
SMILES: CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 226.45

Physical Properties

Property code	Value	Unit	Source
af	0.6061		Cheméo Relay (1.0)
gf	76.52	kJ/mol	Joback Method
hf	-423.76	kJ/mol	Cheméo Relay (1.0)
hfus	26.63	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-7.35		Cheméo Relay (1.0)
logp	6.055		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1446.40		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1449.00		NIST Webbook

rinpol	1449.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1465.10		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	531.31	K	Cheméo Relay (1.0)
tc	685.49	K	Cheméo Relay (1.0)
tf	210.96	K	Cheméo Relay (1.0)
vc	0.896	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.41	J/mol×K	564.16	Joback Method
cpg	721.96	J/mol×K	730.75	Joback Method
cpg	705.63	J/mol×K	702.98	Joback Method
cpg	688.56	J/mol×K	675.22	Joback Method
cpg	670.73	J/mol×K	647.45	Joback Method
cpg	652.10	J/mol×K	619.69	Joback Method
cpg	632.67	J/mol×K	591.92	Joback Method
dvisc	0.0005456	Pa×s	394.62	Joback Method
dvisc	0.0001254	Pa×s	564.16	Joback Method
dvisc	0.0001836	Pa×s	507.65	Joback Method
dvisc	0.0002956	Pa×s	451.13	Joback Method
dvisc	0.0217376	Pa×s	225.08	Joback Method
dvisc	0.0012360	Pa×s	338.11	Joback Method
dvisc	0.0038875	Pa×s	281.59	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3891994&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume