11,15-DIMETHYLHEPTATRIACONTANE

Other names: Heptatriacontane, 11,15-dimethyl
Inchi: InChI=1S/C39H80/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-23-24-25-26-28-30-32-35-39
InchiKey: AXFOBFNPZKQFQZ-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCC
Mol. weight [g/mol]: 549.07

Physical Properties

Property code	Value	Unit	Source
af	1.4399		Cheméo Relay (1.0)
gf	272.62	kJ/mol	Joback Method
hf	-879.24	kJ/mol	Cheméo Relay (1.0)
hfus	89.72	kJ/mol	Joback Method
hvap	183.05	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
log10ws	-13.66		Cheméo Relay (1.0)
logp	15.172		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	408.78	kPa	Joback Method
rinpol	3755.00		NIST Webbook
rinpol	3758.00		NIST Webbook
rinpol	3755.00		NIST Webbook
rinpol	3758.00		NIST Webbook
tb	696.66	K	Cheméo Relay (1.0)
tc	863.33	K	Cheméo Relay (1.0)
tf	299.29	K	Cheméo Relay (1.0)
vc	2.184	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/mol×K	1090.84	Joback Method
cpg	2145.37	J/mol×K	1147.09	Joback Method
cpg	2181.80	J/mol×K	1203.33	Joback Method

cpg	2215.23	J/mol×K	1259.58	Joback Method
cpg	2246.16	J/mol×K	1315.83	Joback Method
cpg	2275.06	J/mol×K	1372.07	Joback Method
cpg	2302.42	J/mol×K	1428.32	Joback Method
dvisc	0.0003958	Pa×s	499.29	Joback Method
dvisc	0.0001036	Pa×s	597.88	Joback Method
dvisc	0.0000396	Pa×s	696.47	Joback Method
dvisc	0.0000192	Pa×s	795.06	Joback Method
dvisc	0.0000110	Pa×s	893.66	Joback Method
dvisc	0.0000070	Pa×s	992.25	Joback Method
dvisc	0.0000048	Pa×s	1090.84	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56987894&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

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