Octacosane, 12,16-dimethyl

Other names: 12,16-Dimethyloctacosane
Inchi: InChI=1S/C30H62/c1-5-7-9-11-13-15-17-19-21-23-26-30(4)28-24-27-29(3)25-22-20-18-1
InchiKey: YHOOTSHMXGAFHF-UHFFFAOYSA-N
Formula: C30H62
SMILES: CCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]: 422.83

Physical Properties

Property code	Value	Unit	Source
af	1.1246		Cheméo Relay (1.0)
gf	196.84	kJ/mol	Joback Method
hf	-694.52	kJ/mol	Cheméo Relay (1.0)
hfus	66.41	kJ/mol	Joback Method
hvap	139.90	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-11.22		Cheméo Relay (1.0)
logp	11.661		Crippen Method
mcvol	433.560	ml/mol	McGowan Method
pc	600.14	kPa	Joback Method
rinpol	2854.00		NIST Webbook
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
rinpol	2857.00		NIST Webbook
rinpol	2856.00		NIST Webbook
tb	640.62	K	Cheméo Relay (1.0)
tc	812.35	K	Cheméo Relay (1.0)
tf	279.91	K	Cheméo Relay (1.0)
vc	1.693	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.72	J/mol×K	884.92	Joback Method
cpg	1509.65	J/mol×K	918.81	Joback Method

cpg	1535.06	J/mol×K	952.69	Joback Method
cpg	1559.02	J/mol×K	986.58	Joback Method
cpg	1581.62	J/mol×K	1020.46	Joback Method
cpg	1602.94	J/mol×K	1054.35	Joback Method
cpg	1623.05	J/mol×K	1088.23	Joback Method
dvisc	0.0017248	Pa×s	397.86	Joback Method
dvisc	0.0004393	Pa×s	479.04	Joback Method
dvisc	0.0001663	Pa×s	560.21	Joback Method
dvisc	0.0000805	Pa×s	641.39	Joback Method
dvisc	0.0000459	Pa×s	722.57	Joback Method
dvisc	0.0000293	Pa×s	803.74	Joback Method
dvisc	0.0000203	Pa×s	884.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R494956&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