Tetratriacontane, 12,16-dimethyl

Inchi: InChI=1S/C46H94/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31
InchiKey: KGDSZZNZGDKTTD-UHFFFAOYSA-N
Formula: C46H94
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]: 647.24

Physical Properties

Property code	Value	Unit	Source
gf	331.56	kJ/mol	Joback Method
hf	-1003.33	kJ/mol	Joback Method
hfus	107.85	kJ/mol	Joback Method
hvap	117.21	kJ/mol	Joback Method
log10ws	-18.59		Crippen Method
logp	17.902		Crippen Method
mcvol	659.000	ml/mol	McGowan Method
pc	316.84	kPa	Joback Method
rinpol	3460.00		NIST Webbook
tb	1251.00	K	Joback Method
tc	1825.60	K	Joback Method
tf	578.18	K	Joback Method
vc	2.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2602.99	J/mol×K	1251.00	Joback Method
cpg	2664.31	J/mol×K	1346.77	Joback Method
cpg	2719.70	J/mol×K	1442.53	Joback Method
cpg	2772.00	J/mol×K	1538.30	Joback Method
cpg	2824.03	J/mol×K	1634.07	Joback Method
cpg	2878.59	J/mol×K	1729.83	Joback Method
cpg	2938.52	J/mol×K	1825.60	Joback Method
dvisc	0.0001195	Pa×s	578.18	Joback Method
dvisc	0.0000318	Pa×s	690.32	Joback Method

dvisc	0.0000122	Pa×s	802.45	Joback Method
dvisc	0.0000059	Pa×s	914.59	Joback Method
dvisc	0.0000034	Pa×s	1026.73	Joback Method
dvisc	0.0000022	Pa×s	1138.86	Joback Method
dvisc	0.0000015	Pa×s	1251.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584633&Units=SI

Legend

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
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

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