Tetratriacontane, 2,20-dimethyl

Inchi: InChI=1S/C46H94/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-28-31-34-37-40-4
InchiKey: RWZQJSLQDKSZSY-UHFFFAOYSA-N
Formula: C46H94
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCC(C)C
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	3494.00		NIST Webbook
rinpol	3494.00		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: 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=R584668&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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