

Tetratriacontane, 2,24-dimethyl

Inchi: InChI=1S/C46H94/c1-5-6-7-8-9-10-11-12-13-14-19-22-25-28-31-34-37-40-43-46(4)44-41
InchiKey: ORSSZVXXONRYHY-UHFFFAOYSA-N
Formula: C46H94
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCCCCCC(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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000122	Paxs	802.45	Joback Method
dvisc	0.0000059	Paxs	914.59	Joback Method
dvisc	0.0000034	Paxs	1026.73	Joback Method
dvisc	0.0000022	Paxs	1138.86	Joback Method
dvisc	0.0000015	Paxs	1251.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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