3,7,11,15-tetramethyl-pentatriacontane

Inchi: InChI=1S/C39H80/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-29-37(4)32
InchiKey: NZUFFAWHTSXINJ-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CC
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	267.74	kJ/mol	Joback Method
hf	-869.41	kJ/mol	Joback Method
hfus	82.67	kJ/mol	Joback Method
hvap	100.86	kJ/mol	Joback Method
log10ws	-15.18		Crippen Method
logp	14.883		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	411.44	kPa	Joback Method
rinpol	3658.00		NIST Webbook
rinpol	3658.00		NIST Webbook
rinpol	3658.00		NIST Webbook
rinpol	3660.00		NIST Webbook
rinpol	3644.00		NIST Webbook
tb	1089.96	K	Joback Method
tc	1415.10	K	Joback Method
tf	469.29	K	Joback Method
vc	2.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.45	J/mol×K	1089.96	Joback Method
cpg	2143.68	J/mol×K	1144.15	Joback Method
cpg	2178.60	J/mol×K	1198.34	Joback Method
cpg	2210.65	J/mol×K	1252.53	Joback Method
cpg	2240.25	J/mol×K	1306.72	Joback Method

cpg	2267.84	J/mol×K	1360.91	Joback Method
cpg	2293.84	J/mol×K	1415.10	Joback Method
dvisc	0.0005981	Pa×s	469.29	Joback Method
dvisc	0.0001218	Pa×s	572.74	Joback Method
dvisc	0.0000404	Pa×s	676.18	Joback Method
dvisc	0.0000179	Pa×s	779.62	Joback Method
dvisc	0.0000096	Pa×s	883.07	Joback Method
dvisc	0.0000059	Pa×s	986.51	Joback Method
dvisc	0.0000040	Pa×s	1089.96	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=R300346&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