

7,11,15,29-tetramethylpentatriacontane

Inchi: InChI=1S/C39H80/c1-7-9-11-22-28-36(3)30-24-20-18-16-14-13-15-17-19-21-25-31-38(5)
InchiKey: PSWAFVCVUQRQZJD-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCC(C)CCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCC
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	3614.00		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/molxK	1089.96	Joback Method
cpg	2267.84	J/molxK	1360.91	Joback Method
cpg	2240.25	J/molxK	1306.72	Joback Method
cpg	2210.65	J/molxK	1252.53	Joback Method
cpg	2178.60	J/molxK	1198.34	Joback Method
cpg	2143.68	J/molxK	1144.15	Joback Method
cpg	2293.84	J/molxK	1415.10	Joback Method
dvisc	0.0000040	Paxs	1089.96	Joback Method
dvisc	0.0000059	Paxs	986.51	Joback Method

dvisc	0.0000096	Paxs	883.07	Joback Method
dvisc	0.0000179	Paxs	779.62	Joback Method
dvisc	0.0000404	Paxs	676.18	Joback Method
dvisc	0.0001218	Paxs	572.74	Joback Method
dvisc	0.0005981	Paxs	469.29	Joback Method

Sources

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=R280490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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