

3,15-dimethylheptatriacontane

Inchi: InChI=1S/C39H80/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-27-30-33-36-39
InchiKey: ZWMSMPPHLSPJDK-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	272.62	kJ/mol	Joback Method
hf	-858.85	kJ/mol	Joback Method
hfus	89.72	kJ/mol	Joback Method
hvap	101.63	kJ/mol	Joback Method
log10ws	-15.66		Crippen Method
logp	15.172		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	408.78	kPa	Joback Method
rinpol	3803.00		NIST Webbook
rinpol	3803.00		NIST Webbook
rinpol	3801.00		NIST Webbook
rinpol	3801.00		NIST Webbook
rinpol	3801.00		NIST Webbook
rinpol	3803.00		NIST Webbook
tb	1090.84	K	Joback Method
tc	1428.32	K	Joback Method
tf	499.29	K	Joback Method
vc	2.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/molxK	1090.84	Joback Method
cpg	2145.37	J/molxK	1147.09	Joback Method
cpg	2181.80	J/molxK	1203.33	Joback Method
cpg	2215.23	J/molxK	1259.58	Joback Method

cpg	2246.16	J/molxK	1315.83	Joback Method
cpg	2275.06	J/molxK	1372.07	Joback Method
cpg	2302.42	J/molxK	1428.32	Joback Method
dvisc	0.0003958	Paxs	499.29	Joback Method
dvisc	0.0001036	Paxs	597.88	Joback Method
dvisc	0.0000396	Paxs	696.47	Joback Method
dvisc	0.0000192	Paxs	795.06	Joback Method
dvisc	0.0000110	Paxs	893.66	Joback Method
dvisc	0.0000070	Paxs	992.25	Joback Method
dvisc	0.0000048	Paxs	1090.84	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=R272276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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