11,15-Dimethylheptatriacontane

Other names: Heptatriacontane, 11,15-dimethyl
Inchi: InChI=1S/C39H80/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-23-24-25-26-28-30-32-35-39
InchiKey: AXFOBFNPZKQFQZ-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCC
Mol. weight [g/mol]: 549.05
CAS: 56987-89-4

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	3755.00		NIST Webbook
rinpol	3758.00		NIST Webbook
rinpol	3755.00		NIST Webbook
rinpol	3758.00		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/mol×K	1090.84	Joback Method
cpg	2145.37	J/mol×K	1147.09	Joback Method
cpg	2181.80	J/mol×K	1203.33	Joback Method
cpg	2215.23	J/mol×K	1259.58	Joback Method

cpg	2246.16	J/mol×K	1315.83	Joback Method
cpg	2275.06	J/mol×K	1372.07	Joback Method
cpg	2302.42	J/mol×K	1428.32	Joback Method
dvisc	0.0003958	Pa×s	499.29	Joback Method
dvisc	0.0001036	Pa×s	597.88	Joback Method
dvisc	0.0000396	Pa×s	696.47	Joback Method
dvisc	0.0000192	Pa×s	795.06	Joback Method
dvisc	0.0000110	Pa×s	893.66	Joback Method
dvisc	0.0000070	Pa×s	992.25	Joback Method
dvisc	0.0000048	Pa×s	1090.84	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=C56987894&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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