Heptacosane, 3,15-dimethyl

Inchi: InChI=1S/C29H60/c1-5-7-8-9-10-11-13-17-20-23-26-29(4)27-24-21-18-15-12-14-16-19-2
InchiKey: AALXPNXCZYISIK-UHFFFAOYSA-N
Formula: C29H60
SMILES: CCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 408.79

Physical Properties

Property code	Value	Unit	Source
gf	188.42	kJ/mol	Joback Method
hf	-652.45	kJ/mol	Joback Method
hfus	63.82	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	-11.48		Crippen Method
logp	11.271		Crippen Method
mcvol	419.470	ml/mol	McGowan Method
pc	629.40	kPa	Joback Method
rinpol	2805.00		NIST Webbook
tb	862.04	K	Joback Method
tc	1057.60	K	Joback Method
tf	386.59	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.45	J/mol×K	862.04	Joback Method
cpg	1441.54	J/mol×K	894.63	Joback Method
cpg	1466.21	J/mol×K	927.23	Joback Method
cpg	1489.54	J/mol×K	959.82	Joback Method
cpg	1511.59	J/mol×K	992.41	Joback Method
cpg	1532.42	J/mol×K	1025.01	Joback Method
cpg	1552.12	J/mol×K	1057.60	Joback Method
dvisc	0.0020179	Pa×s	386.59	Joback Method
dvisc	0.0005120	Pa×s	465.83	Joback Method

dvisc	0.0001936	Pa×s	545.07	Joback Method
dvisc	0.0000937	Pa×s	624.31	Joback Method
dvisc	0.0000534	Pa×s	703.56	Joback Method
dvisc	0.0000341	Pa×s	782.80	Joback Method
dvisc	0.0000236	Pa×s	862.04	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=R555190&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

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