

13,23,27-Trimethyltripentacontane

Inchi:	InChI=1S/C56H114/c1-6-8-10-12-14-16-18-19-20-21-22-23-24-25-26-27-28-29-30-31-33
InchiKey:	ASIOMDGUDKXZBJ-UHFFFAOYSA-N
Formula:	C56H114
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCCCCCC
Mol. weight [g/mol]:	787.50

Physical Properties

Property code	Value	Unit	Source
gf	413.32	kJ/mol	Joback Method
hf	-1215.01	kJ/mol	Joback Method
hfus	130.23	kJ/mol	Joback Method
hvap	139.09	kJ/mol	Joback Method
log10ws	-22.54		Crippen Method
logp	21.659		Crippen Method
mcvol	799.900	ml/mol	McGowan Method
pc	231.67	kPa	Joback Method
rinpol	5363.00		NIST Webbook
tb	1479.36	K	Joback Method
tc	2842.55	K	Joback Method
tf	675.88	K	Joback Method
vc	3.154	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3329.51	J/molxK	1479.36	Joback Method
cpg	3480.83	J/molxK	1706.56	Joback Method
cpg	3664.62	J/molxK	1933.76	Joback Method
cpg	3926.88	J/molxK	2160.95	Joback Method
cpg	4313.61	J/molxK	2388.15	Joback Method
cpg	4870.80	J/molxK	2615.35	Joback Method
cpg	5644.46	J/molxK	2842.55	Joback Method
dvisc	0.0000228	Paxs	675.88	Joback Method
dvisc	0.0000056	Paxs	809.79	Joback Method

dvisc	0.0000021	Paxs	943.71	Joback Method
dvisc	0.0000010	Paxs	1077.62	Joback Method
dvisc	0.0000005	Paxs	1211.53	Joback Method
dvisc	0.0000003	Paxs	1345.45	Joback Method
dvisc	0.0000002	Paxs	1479.36	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=R337605&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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