

Mint sulfide

Inchi: InChI=1S/C15H24S/c1-9(2)11-8-12-15(4)7-5-6-10(3)14(16-12)13(11)15/h9,11-14H,3,5-8
InchiKey: ALHAUSWZZFZREA-CQYKSGMSSA-N
Formula: C15H24S
SMILES: C=C1CCCC2(C)C3CC(C(C)C)C2C1S3
Mol. weight [g/mol]: 236.42

Physical Properties

Property code	Value	Unit	Source
gf	303.06	kJ/mol	Joback Method
hf	-48.07	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.509		Crippen Method
mcvol	201.680	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1746.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2105.00		NIST Webbook
tb	608.81	K	Joback Method
tc	839.95	K	Joback Method
tf	403.14	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.71	J/molxK	608.81	Joback Method
cpg	582.66	J/molxK	647.33	Joback Method
cpg	604.14	J/molxK	685.86	Joback Method

cpg	624.36	J/mol×K	724.38	Joback Method
cpg	643.55	J/mol×K	762.90	Joback Method
cpg	661.91	J/mol×K	801.43	Joback Method
cpg	679.65	J/mol×K	839.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R604445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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