Methitural

Inchi: InChI=1S/C12H20N2O2S2/c1-4-5-8(2)12(6-7-18-3)9(15)13-11(17)14-10(12)16/h8H,4-7H
InchiKey: KEMCRVSPPRNENL-UHFFFAOYSA-N
Formula: C12H20N2O2S2
SMILES: CCCC(C)C1(CCSC)C(=O)N=C(S)NC1=O
Mol. weight [g/mol]: 288.43
CAS: 467-43-6

Physical Properties

Property code	Value	Unit	Source
gf	108.83	kJ/mol	Joback Method
hf	-266.69	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	77.17	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.104		Crippen Method
mcvol	220.580	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	866.98	K	Joback Method
tc	1139.38	K	Joback Method
tf	638.43	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.40	J/mol×K	866.98	Joback Method
cpg	701.61	J/mol×K	912.38	Joback Method
cpg	718.51	J/mol×K	957.78	Joback Method
cpg	734.16	J/mol×K	1003.18	Joback Method
cpg	748.59	J/mol×K	1048.58	Joback Method
cpg	761.84	J/mol×K	1093.98	Joback Method

cpg	773.96	J/mol×K	1139.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C467436&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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