Acetohexamide, N-methyl-

Inchi: InChI=1S/C16H22N2O4S/c1-12(19)13-8-10-15(11-9-13)23(21,22)18(2)16(20)17-14-6-4-3
InchiKey: LJUVADVEZRRERT-UHFFFAOYSA-N
Formula: C16H22N2O4S
SMILES: CC(=O)c1ccc(S(=O)(=O)N(C)C(=O)NC2CCCCC2)cc1
Mol. weight [g/mol]: 338.42

Physical Properties

Property code	Value	Unit	Source
gf	-315.14	kJ/mol	Joback Method
hf	-651.70	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	95.18	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	2.552		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	834.82	K	Joback Method
tc	1058.54	K	Joback Method
tf	539.95	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.78	J/mol×K	834.82	Joback Method
cpg	789.87	J/mol×K	872.11	Joback Method
cpg	803.45	J/mol×K	909.39	Joback Method
cpg	815.58	J/mol×K	946.68	Joback Method
cpg	826.29	J/mol×K	983.97	Joback Method
cpg	835.65	J/mol×K	1021.26	Joback Method
cpg	843.69	J/mol×K	1058.54	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=U374403&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