Urea, 1-methyl-3-methylsulfonyl-

Inchi: InChI=1S/C3H8N2O3S/c1-4-3(6)5-9(2,7)8/h1-2H3,(H2,4,5,6)
InchiKey: GQSFASWYVBMKSL-UHFFFAOYSA-N
Formula: C3H8N2O3S
SMILES: CNC(=O)NS(C)(=O)=O
Mol. weight [g/mol]: 152.17
CAS: 33024-69-0

Physical Properties

Property code	Value	Unit	Source
gf	-444.30	kJ/mol	Joback Method
hf	-564.24	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	60.53	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	-1.125		Crippen Method
mcvol	102.750	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
tb	470.03	K	Joback Method
tc	656.06	K	Joback Method
tf	317.38	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.94	J/mol×K	470.03	Joback Method
cpg	220.62	J/mol×K	501.03	Joback Method
cpg	228.93	J/mol×K	532.04	Joback Method
cpg	236.87	J/mol×K	563.04	Joback Method
cpg	244.43	J/mol×K	594.05	Joback Method
cpg	251.60	J/mol×K	625.05	Joback Method
cpg	258.38	J/mol×K	656.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33024690&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume