Urea, 1,3-bis (2,2,2-trifluoroethyl)-

Inchi: InChI=1S/C5H6F6N2O/c6-4(7,8)1-12-3(14)13-2-5(9,10)11/h1-2H2,(H2,12,13,14)
InchiKey: NLTKGUVQZXMRSZ-UHFFFAOYSA-N
Formula: C5H6F6N2O
SMILES: O=C(NCC(F)(F)F)NCC(F)(F)F
Mol. weight [g/mol]: 224.10
CAS: 406-11-1

Physical Properties

Property code	Value	Unit	Source
gf	-1122.10	kJ/mol	Joback Method
hf	-1346.33	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.410		Crippen Method
mcvol	113.460	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	457.17	K	Joback Method
tc	613.53	K	Joback Method
tf	309.74	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.09	J/mol×K	457.17	Joback Method
cpg	285.48	J/mol×K	483.23	Joback Method
cpg	294.29	J/mol×K	509.29	Joback Method
cpg	302.56	J/mol×K	535.35	Joback Method
cpg	310.30	J/mol×K	561.41	Joback Method
cpg	317.54	J/mol×K	587.47	Joback Method
cpg	324.30	J/mol×K	613.53	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=C406111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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