

(2S)-Bornane-10,2-sultam

Inchi:	InChI=1S/C10H17NO2S/c1-9(2)7-3-4-10(9)6-14(12,13)11-8(10)5-7/h7-8,11H,3-6H2,1-2H
InchiKey:	DPJYJNYDJOJNO-JEUQWKINSA-N
Formula:	C10H17NO2S
SMILES:	CC1(C)C2CCC13CS(=O)(=O)NC3C2
Mol. weight [g/mol]:	215.31
CAS:	108448-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-189.31	kJ/mol	Joback Method
hf	-439.50	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.114		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	523.88	K	Joback Method
tc	745.67	K	Joback Method
tf	488.96	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.22	J/molxK	523.88	Joback Method
cpg	417.52	J/molxK	560.85	Joback Method
cpg	435.20	J/molxK	597.81	Joback Method
cpg	451.53	J/molxK	634.78	Joback Method
cpg	466.79	J/molxK	671.74	Joback Method
cpg	481.25	J/molxK	708.71	Joback Method
cpg	495.16	J/molxK	745.67	Joback Method

Sources

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=C108448777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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