

Propanesulfonylacetone nitrile

Inchi:	InChI=1S/C5H9NO2S/c1-2-4-9(7,8)5-3-6/h2,4-5H2,1H3
InchiKey:	OVGCBSNAUREBIE-UHFFFAOYSA-N
Formula:	C5H9NO2S
SMILES:	CCCS(=O)(=O)CC#N
Mol. weight [g/mol]:	147.19
CAS:	175137-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-344.14	kJ/mol	Joback Method
hf	-435.00	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	55.84	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.335		Crippen Method
mvol	110.780	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	463.66	K	Joback Method
tc	649.95	K	Joback Method
tf	249.66	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/molxK	463.66	Joback Method
cpg	230.15	J/molxK	494.71	Joback Method
cpg	238.72	J/molxK	525.76	Joback Method
cpg	246.93	J/molxK	556.80	Joback Method
cpg	254.78	J/molxK	587.85	Joback Method
cpg	262.27	J/molxK	618.90	Joback Method
cpg	269.38	J/molxK	649.95	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=C175137618&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
mccvol:	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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