

Sulforaphane nitrile

Other names:	5-(Methylsulfinyl)pentanenitrile
Inchi:	InChI=1S/C6H11NOS/c1-9(8)6-4-2-3-5-7/h2-4,6H2,1H3
InchiKey:	FGYQUFZANKOISC-UHFFFAOYSA-N
Formula:	C6H11NOS
SMILES:	CS(=O)CCCCC#N
Mol. weight [g/mol]:	145.22
CAS:	61121-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-84.89	kJ/mol	Joback Method
hf	-208.03	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	1.059		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	497.04	K	Joback Method
tc	693.88	K	Joback Method
tf	258.85	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.63	J/molxK	497.04	Joback Method
cpg	257.62	J/molxK	529.85	Joback Method
cpg	267.18	J/molxK	562.65	Joback Method
cpg	276.30	J/molxK	595.46	Joback Method
cpg	284.98	J/molxK	628.27	Joback Method
cpg	293.22	J/molxK	661.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61121662&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

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

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