

Butyl methylaminodithiocarbamate

Inchi:	InChI=1S/C6H13NS2/c1-3-4-5-9-6(8)7-2/h3-5H2,1-2H3,(H,7,8)
InchiKey:	XSVAFMVYJMBMRO-UHFFFAOYSA-N
Formula:	C6H13NS2
SMILES:	CCCCSC(=S)NC
Mol. weight [g/mol]:	163.30

Physical Properties

Property code	Value	Unit	Source
gf	239.21	kJ/mol	Joback Method
hf	74.67	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	48.93	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.024		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	525.67	K	Joback Method
tc	744.38	K	Joback Method
tf	278.71	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.82	J/molxK	525.67	Joback Method
cpg	292.35	J/molxK	562.12	Joback Method

cpg	303.17	J/mol×K	598.57	Joback Method
cpg	313.31	J/mol×K	635.03	Joback Method
cpg	322.81	J/mol×K	671.48	Joback Method
cpg	331.74	J/mol×K	707.93	Joback Method
cpg	340.11	J/mol×K	744.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R11193&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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