Di(isobutyl)dithiocarbamic acid

Inchi: InChI=1S/C9H19NS2/c1-7(2)5-10(9(11)12)6-8(3)4/h7-8H,5-6H2,1-4H3,(H,11,12)
InchiKey: CBQPQMSTIARRSA-UHFFFAOYSA-N
Formula: C9H19NS2
SMILES: CC(C)CN(CC(C)C)C(=S)S
Mol. weight [g/mol]: 205.38
CAS: 7283-77-4

Physical Properties

Property code	Value	Unit	Source
gf	277.25	kJ/mol	Joback Method
hf	-67.60 ± 2.40	kJ/mol	NIST Webbook
hfus	23.69	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.815		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	549.78	K	Joback Method
tc	764.09	K	Joback Method
tf	264.39	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.99	J/mol×K	549.78	Joback Method
cpg	417.57	J/mol×K	585.50	Joback Method
cpg	432.16	J/mol×K	621.22	Joback Method
cpg	445.82	J/mol×K	656.93	Joback Method
cpg	458.62	J/mol×K	692.65	Joback Method
cpg	470.63	J/mol×K	728.37	Joback Method
cpg	481.92	J/mol×K	764.09	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=C7283774&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