Carbamodithioic acid, dibutyl-, methyl ester

Inchi: InChI=1S/C10H21NS2/c1-4-6-8-11(9-7-5-2)10(12)13-3/h4-9H2,1-3H3
InchiKey: RTBHUIONIQBBGN-UHFFFAOYSA-N
Formula: C10H21NS2
SMILES: CCCCN(CCCC)C(=S)SC
Mol. weight [g/mol]: 219.41
CAS: 38351-44-9

Physical Properties

Property code	Value	Unit	Source
gf	294.28	kJ/mol	Joback Method
hf	6.17	kJ/mol	Joback Method
hfus	33.41	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.537		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
tb	579.46	K	Joback Method
tc	781.46	K	Joback Method
tf	303.60	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.25	J/mol×K	579.46	Joback Method
cpg	467.73	J/mol×K	613.13	Joback Method
cpg	482.32	J/mol×K	646.79	Joback Method
cpg	496.08	J/mol×K	680.46	Joback Method
cpg	509.05	J/mol×K	714.13	Joback Method
cpg	521.29	J/mol×K	747.79	Joback Method
cpg	532.84	J/mol×K	781.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38351449&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