Carbamothioic acid, N-butyl-N-(2-propynyl), s-ethyl ester

Inchi: InChI=1S/C10H17NOS/c1-4-7-9-11(8-5-2)10(12)13-6-3/h2H,4,6-9H2,1,3H3
InchiKey: BDKSDZPMBZXPED-UHFFFAOYSA-N
Formula: C10H17NOS
SMILES: C#CCN(CCCC)C(=O)SCC
Mol. weight [g/mol]: 199.31
CAS: 59300-35-5

Physical Properties

Property code	Value	Unit	Source
gf	271.37	kJ/mol	Joback Method
hf	38.99	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.595		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	553.41	K	Joback Method
tc	754.28	K	Joback Method
tf	366.23	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.71	J/mol×K	553.41	Joback Method
cpg	410.92	J/mol×K	586.89	Joback Method
cpg	424.34	J/mol×K	620.37	Joback Method
cpg	437.02	J/mol×K	653.85	Joback Method
cpg	448.99	J/mol×K	687.33	Joback Method
cpg	460.26	J/mol×K	720.80	Joback Method
cpg	470.87	J/mol×K	754.28	Joback Method
hsubt	82.10	kJ/mol	305.50	NIST Webbook

Sources

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=C59300355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt:	Enthalpy of sublimation at a given temperature
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