Carbamothioic acid, bis(2-methylpropyl)-, S-ethyl ester

Other names: Anelda
Bis(2-methylpropyl)carbamothioic acid S-ethyl ester
Butilate
Butylate
Carbamic acid, diisobutylthio-, S-ethyl ester
Carbamothioic acid, N,N-bis(2-methylpropyl)-, S-ethyl ester
Diisobutylthiocarbamic acid S-ethyl ester
Diisocarb
Ethyl N,N-diisobutylthiocarbamate
Ethyl N,N-diisobutylthiolcarbamate
R 1910
S-Ethyl N,N-diisobutyl thiocarbamate
S-Ethyl N,N-diisobutyl thiolcarbamate
S-Ethyl bis(2-methylpropyl)carbamothioate
Stauffer R-1,910
Stauffer R-1910
Sutan
s-Ethyl diisobutyl thiocarbamate

Inchi: InChI=1S/C11H23NOS/c1-6-14-11(13)12(7-9(2)3)8-10(4)5/h9-10H,6-8H2,1-5H3

InchiKey: BMTAFVWTTFSTOG-UHFFFAOYSA-N

Formula: C11H23NOS

SMILES: CCSC(=O)N(CC(C)C)CC(C)C

Mol. weight [g/mol]: 217.37

CAS: 2008-41-5

Physical Properties

Property code	Value	Unit	Source
gf	51.84	kJ/mol	Joback Method
hf	-284.11	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	54.91	kJ/mol	Joback Method
log10ws	-3.68		Aqueous Solubility Prediction Method
log10ws	-3.68		Estimated Solubility Method
logp	3.473		Crippen Method
mcvol	193.750	ml/mol	McGowan Method

pc	2104.20	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	585.29	K	Joback Method
tc	778.91	K	Joback Method
tf	300.53	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.98	J/mol×K	585.29	Joback Method
cpg	502.67	J/mol×K	617.56	Joback Method
cpg	518.50	J/mol×K	649.83	Joback Method
cpg	533.49	J/mol×K	682.10	Joback Method
cpg	547.67	J/mol×K	714.37	Joback Method
cpg	561.06	J/mol×K	746.64	Joback Method
cpg	573.69	J/mol×K	778.91	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2008415&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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