Carbamic acid, [2-(thiocarbamoyl)ethyl]-,benzyl ester

Inchi: InChI=1S/C11H14N2O2S/c12-10(16)6-7-13-11(14)15-8-9-4-2-1-3-5-9/h1-5H,6-8H2,(H2,1

InchiKey: QHEDAKTWMKKBTE-UHFFFAOYSA-N

Formula: C11H14N2O2S

SMILES: NC(=S)CCNC(=O)OCc1ccccc1

Mol. weight [g/mol]: 238.31

CAS: 77152-98-8

Physical Properties

Property code	Value	Unit	Source
gf	193.13	kJ/mol	Joback Method
hf	-44.88	kJ/mol	Joback Method
hfus	35.97	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	1.589		Crippen Method
mcvol	181.540	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	746.79	K	Joback Method
tc	982.59	K	Joback Method
tf	482.50	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.54	J/mol×K	746.79	Joback Method
cpg	493.26	J/mol×K	786.09	Joback Method
cpg	504.11	J/mol×K	825.39	Joback Method
cpg	514.14	J/mol×K	864.69	Joback Method
cpg	523.45	J/mol×K	903.99	Joback Method
cpg	532.10	J/mol×K	943.29	Joback Method
cpg	540.17	J/mol×K	982.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77152988&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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