Carbamic acid, n-(2-cyanoethyl)-, phenylmethyl ester

Inchi: InChI=1S/C11H12N2O2/c12-7-4-8-13-11(14)15-9-10-5-2-1-3-6-10/h1-3,5-6H,4,8-9H2,(H
InchiKey: KTPATXCSHZCTMY-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: N#CCCNC(=O)OCc1ccccc1
Mol. weight [g/mol]: 204.23
CAS: 18877-96-8

Physical Properties

Property code	Value	Unit	Source
gf	142.80	kJ/mol	Joback Method
hf	-60.29	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.826		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	706.30	K	Joback Method
tc	928.33	K	Joback Method
tf	429.96	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.89	J/mol×K	706.30	Joback Method
cpg	431.32	J/mol×K	743.31	Joback Method
cpg	441.92	J/mol×K	780.31	Joback Method
cpg	451.72	J/mol×K	817.32	Joback Method
cpg	460.74	J/mol×K	854.32	Joback Method
cpg	469.01	J/mol×K	891.33	Joback Method
cpg	476.55	J/mol×K	928.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18877968&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