Propanamide, 2-(acetylamino)-3-methoxy-N-(phenylmethyl)-, (2R)-

Other names: Lacosamide
Inchi: InChI=1S/C13H18N2O3/c1-10(16)15-12(9-18-2)13(17)14-8-11-6-4-3-5-7-11/h3-7,12H,8-
InchiKey: VPPJLAIAVCUEMN-UHFFFAOYSA-N
Formula: C13H18N2O3
SMILES: COCC(NC(C)=O)C(=O)NCc1ccccc1
Mol. weight [g/mol]: 250.29
CAS: 175481-36-4

Physical Properties

Property code	Value	Unit	Source
gf	-15.51	kJ/mol	Joback Method
hf	-330.84	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	75.19	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	0.454		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2074.20		NIST Webbook
rinpol	2074.20		NIST Webbook
tb	753.58	K	Joback Method
tc	966.68	K	Joback Method
tf	475.10	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.21	J/mol×K	753.58	Joback Method
cpg	581.67	J/mol×K	789.10	Joback Method
cpg	594.14	J/mol×K	824.61	Joback Method
cpg	605.66	J/mol×K	860.13	Joback Method
cpg	616.25	J/mol×K	895.64	Joback Method
cpg	625.95	J/mol×K	931.16	Joback Method

cpg	634.80	J/mol×K	966.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175481364&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume