Ethyl 3-(benzyl-acetamino)propanoate

Other names: Alanine, N-(phenylmethyl)-N-acetyl, ethyl ester
3-Benzyl-acetaminopropionic acid ethyl ester
N-Benzyl-N-acetyl-3-aminopropionic acid, Ethyl ester
Ethyl 3-(acetyl-benzyl-amino)propanoate
Inchi: InChI=1S/C14H19NO3/c1-3-18-14(17)9-10-15(12(2)16)11-13-7-5-4-6-8-13/h4-8H,3,9-11
InchiKey: QCNIWBXYUVRCTE-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: CCOC(=O)CCN(Cc1ccccc1)C(C)=O
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-72.65	kJ/mol	Joback Method
hf	-385.61	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.988		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2016.00		NIST Webbook
tb	689.00	K	Joback Method
tc	893.48	K	Joback Method
tf	428.52	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.17	J/mol×K	689.00	Joback Method
cpg	568.23	J/mol×K	723.08	Joback Method
cpg	582.32	J/mol×K	757.16	Joback Method
cpg	595.47	J/mol×K	791.24	Joback Method
cpg	607.72	J/mol×K	825.32	Joback Method

cpg	619.10	J/mol×K	859.40	Joback Method
cpg	629.65	J/mol×K	893.48	Joback Method

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=U373073&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
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