(.+/-.)-BDB

Inchi: InChI=1S/C11H15NO2/c1-2-9(12)5-8-3-4-10-11(6-8)14-7-13-10/h3-4,6,9H,2,5,7,12H2,1H
InchiKey: VHMRXGAIDDCGDU-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCC(N)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 193.24
CAS: 107447-03-0

Physical Properties

Property code	Value	Unit	Source
gf	95.12	kJ/mol	Joback Method
hf	-199.13	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.695		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1619.50		NIST Webbook
rinpol	1619.50		NIST Webbook
tb	625.12	K	Joback Method
tc	855.07	K	Joback Method
tf	408.77	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.69	J/mol×K	625.12	Joback Method
cpg	419.95	J/mol×K	663.45	Joback Method
cpg	433.22	J/mol×K	701.77	Joback Method
cpg	445.57	J/mol×K	740.10	Joback Method
cpg	457.08	J/mol×K	778.42	Joback Method
cpg	467.83	J/mol×K	816.75	Joback Method
cpg	477.88	J/mol×K	855.07	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=C107447030&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