(.+/-.)-MDEA

Inchi: InChI=1S/C12H17NO2/c1-3-13-9(2)6-10-4-5-11-12(7-10)15-8-14-11/h4-5,7,9,13H,3,6,8H
InchiKey: PVXVWWANJIWJOO-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCNC(C)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 207.27
CAS: 82801-81-8

Physical Properties

Property code	Value	Unit	Source
gf	126.48	kJ/mol	Joback Method
hf	-200.09	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.956		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1596.40		NIST Webbook
rinpol	1596.40		NIST Webbook
tb	625.64	K	Joback Method
tc	843.18	K	Joback Method
tf	389.44	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.14	J/mol×K	625.64	Joback Method
cpg	460.34	J/mol×K	661.90	Joback Method
cpg	474.55	J/mol×K	698.15	Joback Method
cpg	487.84	J/mol×K	734.41	Joback Method
cpg	500.28	J/mol×K	770.66	Joback Method
cpg	511.93	J/mol×K	806.92	Joback Method
cpg	522.85	J/mol×K	843.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82801818&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