2-Isobutylbenzoxazone-4

Inchi: InChI=1S/C12H15NO2/c1-8(2)7-11-13-12(14)9-5-3-4-6-10(9)15-11/h3-6,8,11H,7H2,1-2H
InchiKey: XPBPOARBCZQXPO-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: CC(C)CC1NC(=O)c2ccccc2O1
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
gf	78.15	kJ/mol	Joback Method
hf	-236.48	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	60.46	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.181		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	659.51	K	Joback Method
tc	903.13	K	Joback Method
tf	463.18	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.25	J/mol×K	659.51	Joback Method
cpg	458.24	J/mol×K	700.11	Joback Method
cpg	474.06	J/mol×K	740.72	Joback Method
cpg	488.73	J/mol×K	781.32	Joback Method
cpg	502.27	J/mol×K	821.92	Joback Method
cpg	514.70	J/mol×K	862.52	Joback Method
cpg	526.04	J/mol×K	903.13	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=B6000036&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume