7-Difluoromethoxy-2,3-dihydro-5-phenyl-1H-1,4-b

Inchi: InChI=1S/C16H12F2N2O2/c17-16(18)22-11-6-7-13-12(8-11)15(19-9-14(21)20-13)10-4-2
InchiKey: WMEDSEKKSZGVOM-UHFFFAOYSA-N
Formula: C16H12F2N2O2
SMILES: O=C1CN=C(c2ccccc2)c2cc(OC(F)F)ccc2N1
Mol. weight [g/mol]: 302.28
CAS: 55384-53-7

Physical Properties

Property code	Value	Unit	Source
gf	-61.17	kJ/mol	Joback Method
hf	-354.96	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.078		Crippen Method
mcvol	204.560	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	843.48	K	Joback Method
tc	1104.23	K	Joback Method
tf	629.58	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.26	J/mol×K	843.48	Joback Method
cpg	634.28	J/mol×K	886.94	Joback Method
cpg	646.46	J/mol×K	930.40	Joback Method
cpg	656.80	J/mol×K	973.86	Joback Method
cpg	665.27	J/mol×K	1017.32	Joback Method
cpg	671.88	J/mol×K	1060.77	Joback Method
cpg	676.61	J/mol×K	1104.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55384537&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume