4,4'-Difluorobenzil

Inchi:	InChI=1S/C14H8F2O2/c15-11-5-1-9(2-6-11)13(17)14(18)10-3-7-12(16)8-4-10/h1-8H
InchiKey:	BRKULQOUSCHDGS-UHFFFAOYSA-N
Formula:	C14H8F2O2
SMILES:	O=C(C(=O)c1ccc(F)cc1)c1ccc(F)cc1
Mol. weight [g/mol]:	246.21
CAS:	579-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-374.90	kJ/mol	Joback Method
hf	-499.55	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	64.49	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.030		Crippen Method
mcvol	167.280	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	689.32	K	Joback Method
tc	921.03	K	Joback Method
tf	426.46	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.84	J/mol×K	689.32	Joback Method
cpg	430.91	J/mol×K	727.94	Joback Method
cpg	441.99	J/mol×K	766.56	Joback Method
cpg	452.12	J/mol×K	805.17	Joback Method
cpg	461.35	J/mol×K	843.79	Joback Method
cpg	469.75	J/mol×K	882.41	Joback Method
cpg	477.35	J/mol×K	921.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C579395&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

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

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