

Dibenzyl, 4,4'-difluoro-2,2'-dinitro-

Other names:	4,4'-difluoro-2,2'-dinitrobibenzyl
Inchi:	InChI=1S/C14H10F2N2O4/c15-11-5-3-9(13(7-11)17(19)20)1-2-10-4-6-12(16)8-14(10)18
InchiKey:	NRDWMCMPPQKQMY-UHFFFAOYSA-N
Formula:	C14H10F2N2O4
SMILES:	O=[N+]([O-])c1cc(F)ccc1CCc1ccc(F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	308.24
CAS:	50618-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-65.22	kJ/mol	Joback Method
hf	-318.85	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	3.566		Crippen Method
mcvol	198.980	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	895.22	K	Joback Method
tc	1152.50	K	Joback Method
tf	638.86	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.19	J/molxK	895.22	Joback Method
cpg	586.25	J/molxK	938.10	Joback Method
cpg	595.29	J/molxK	980.98	Joback Method
cpg	603.38	J/molxK	1023.86	Joback Method
cpg	610.60	J/molxK	1066.74	Joback Method
cpg	617.02	J/molxK	1109.62	Joback Method
cpg	622.71	J/molxK	1152.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50618923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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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