

Isophthalic acid, 2-bromo-4-fluorophenyl propyl ester

Inchi:	InChI=1S/C17H14BrFO4/c1-2-8-22-16(20)11-4-3-5-12(9-11)17(21)23-15-7-6-13(19)10-1
InchiKey:	CDIHJJIXEQBVML-UHFFFAOYSA-N
Formula:	C17H14BrFO4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccc(F)cc2Br)c1
Mol. weight [g/mol]:	381.19

Physical Properties

Property code	Value	Unit	Source
gf	-360.14	kJ/mol	Joback Method
hf	-614.94	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	83.90	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.374		Crippen Method
mcvol	237.020	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	874.67	K	Joback Method
tc	1109.03	K	Joback Method
tf	576.46	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.74	J/molxK	874.67	Joback Method
cpg	660.85	J/molxK	913.73	Joback Method
cpg	670.81	J/molxK	952.79	Joback Method
cpg	679.67	J/molxK	991.85	Joback Method
cpg	687.45	J/molxK	1030.91	Joback Method
cpg	694.17	J/molxK	1069.97	Joback Method
cpg	699.87	J/molxK	1109.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U344394&Units=SI

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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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