

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

Inchi:	InChI=1S/C22H24BrFO4/c1-2-3-4-5-6-7-13-27-21(25)16-9-8-10-17(14-16)22(26)28-20-1
InchiKey:	ALYMGWWHXHFHFO-UHFFFAOYSA-N
Formula:	C22H24BrFO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(F)cc2Br)c1
Mol. weight [g/mol]:	451.33

Physical Properties

Property code	Value	Unit	Source
gf	-318.04	kJ/mol	Joback Method
hf	-718.14	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	95.03	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	6.325		Crippen Method
mvol	307.470	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	989.07	K	Joback Method
tc	1218.90	K	Joback Method
tf	632.81	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.82	J/mol×K	989.07	Joback Method
cpg	947.67	J/mol×K	1027.37	Joback Method
cpg	958.24	J/mol×K	1065.68	Joback Method
cpg	967.58	J/mol×K	1103.98	Joback Method
cpg	975.75	J/mol×K	1142.29	Joback Method
cpg	982.77	J/mol×K	1180.59	Joback Method
cpg	988.71	J/mol×K	1218.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344401&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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