

Phthalic acid, 2-bromo-5-fluorobenzyl propyl ester

Inchi:	InChI=1S/C18H16BrFO4/c1-2-9-23-17(21)14-5-3-4-6-15(14)18(22)24-11-12-10-13(20)7-
InchiKey:	VQHGYQOTBCNAIR-UHFFFAOYSA-N
Formula:	C18H16BrFO4
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	395.22

Physical Properties

Property code	Value	Unit	Source
gf	-351.72	kJ/mol	Joback Method
hf	-635.58	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.512		Crippen Method
mcvol	251.110	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2899.00		NIST Webbook
rinpol	2899.00		NIST Webbook
tb	897.55	K	Joback Method
tc	1129.47	K	Joback Method
tf	587.73	K	Joback Method
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.53	J/mol×K	897.55	Joback Method
cpg	716.83	J/mol×K	936.20	Joback Method
cpg	726.98	J/mol×K	974.86	Joback Method
cpg	736.00	J/mol×K	1013.51	Joback Method
cpg	743.92	J/mol×K	1052.16	Joback Method
cpg	750.77	J/mol×K	1090.82	Joback Method
cpg	756.59	J/mol×K	1129.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382505&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
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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