

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

Inchi:	InChI=1S/C24H28BrFO4/c1-2-3-4-5-6-7-10-15-29-23(27)20-11-8-9-12-21(20)24(28)30-1
InchiKey:	NDDMTOTVIGOBHV-UHFFFAOYSA-N
Formula:	C24H28BrFO4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	479.38

Physical Properties

Property code	Value	Unit	Source
gf	-301.20	kJ/mol	Joback Method
hf	-759.42	kJ/mol	Joback Method
hfus	58.77	kJ/mol	Joback Method
hvap	99.49	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	6.853		Crippen Method
mcvol	335.650	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpola	3496.00		NIST Webbook
rinpola	3496.00		NIST Webbook
tb	1034.83	K	Joback Method
tc	1268.87	K	Joback Method
tf	655.35	K	Joback Method
vc	1.292	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.49	J/molxK	1034.83	Joback Method
cpg	1066.55	J/molxK	1073.84	Joback Method
cpg	1077.26	J/molxK	1112.84	Joback Method
cpg	1086.66	J/molxK	1151.85	Joback Method
cpg	1094.81	J/molxK	1190.86	Joback Method
cpg	1101.78	J/molxK	1229.86	Joback Method
cpg	1107.62	J/molxK	1268.87	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=U382512&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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