Terephthalic acid, 2-bromo-5-fluorobenzyl pentyl ester

Inchi: InChI=1S/C20H20BrFO4/c1-2-3-4-11-25-19(23)14-5-7-15(8-6-14)20(24)26-13-16-12-17(

InchiKey: GTRPZHHWVYSOGD-UHFFFAOYSA-N

Formula: C20H20BrFO4

SMILES: CCCCCOC(=O)c1ccc(C(=O)OCc2cc(F)ccc2Br)cc1

Mol. weight [g/mol]: 423.27

Physical Properties

Property code	Value	Unit	Source
gf	-334.88	kJ/mol	Joback Method
hf	-676.86	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	5.292		Crippen Method
mcvol	279.290	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	943.31	K	Joback Method
tc	1172.56	K	Joback Method
tf	610.27	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.36	J/mol×K	943.31	Joback Method
cpg	830.97	J/mol×K	981.52	Joback Method
cpg	841.38	J/mol×K	1019.73	Joback Method
cpg	850.61	J/mol×K	1057.94	Joback Method
cpg	858.70	J/mol×K	1096.15	Joback Method
cpg	865.70	J/mol×K	1134.35	Joback Method
cpg	871.64	J/mol×K	1172.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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