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

Inchi: InChI=1S/C17H14BrFO4/c1-2-22-16(20)11-3-5-12(6-4-11)17(21)23-10-13-9-14(19)7-8-15

InchiKey: HSJQMEXXGUOFDG-UHFFFAOYSA-N

Formula: C17H14BrFO4

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

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	-5.98		Crippen Method
logp	4.122		Crippen Method
mcvol	237.020	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		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/mol×K	874.67	Joback Method
cpg	660.85	J/mol×K	913.73	Joback Method
cpg	670.81	J/mol×K	952.79	Joback Method
cpg	679.67	J/mol×K	991.85	Joback Method
cpg	687.45	J/mol×K	1030.91	Joback Method
cpg	694.17	J/mol×K	1069.97	Joback Method
cpg	699.87	J/mol×K	1109.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416063&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
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