Terephthalic acid, 4-bromo-2,6-difluorobenzyl ethyl ester

Inchi: InChI=1S/C17H13BrF2O4/c1-2-23-16(21)10-3-5-11(6-4-10)17(22)24-9-13-14(19)7-12(18

InchiKey: NGELAPXOKTXNOP-UHFFFAOYSA-N

Formula: C17H13BrF2O4

SMILES: CCOC(=O)c1ccc(C(=O)OCc2c(F)cc(Br)cc2F)cc1

Mol. weight [g/mol]: 399.18

Physical Properties

Property code	Value	Unit	Source
gf	-564.58	kJ/mol	Joback Method
hf	-822.52	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	83.75	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.261		Crippen Method
mcvol	238.790	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	878.92	K	Joback Method
tc	1106.73	K	Joback Method
tf	589.57	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.49	J/mol×K	878.92	Joback Method
cpg	666.05	J/mol×K	916.89	Joback Method
cpg	675.52	J/mol×K	954.86	Joback Method
cpg	683.94	J/mol×K	992.83	Joback Method
cpg	691.32	J/mol×K	1030.80	Joback Method
cpg	697.67	J/mol×K	1068.77	Joback Method
cpg	703.02	J/mol×K	1106.73	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=U416028&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