Terephthalic acid, isobutyl 2-fluoro-5-nitrobenzyl ester

Inchi: InChI=1S/C19H18FNO6/c1-12(2)10-26-18(22)13-3-5-14(6-4-13)19(23)27-11-15-9-16(21(

InchiKey: CPJTWJZKEZCMRD-UHFFFAOYSA-N

Formula: C19H18FNO6

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2cc([N+](=O)[O-])ccc2F)cc1

Mol. weight [g/mol]: 375.35

Physical Properties

Property code	Value	Unit	Source
gf	-324.51	kJ/mol	Joback Method
hf	-698.59	kJ/mol	Joback Method
hfus	48.37	kJ/mol	Joback Method
hvap	98.12	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	3.904		Crippen Method
mcvol	265.120	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	1005.67	K	Joback Method
tc	1248.66	K	Joback Method
tf	667.81	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.68	J/mol×K	1005.67	Joback Method
cpg	833.01	J/mol×K	1046.17	Joback Method
cpg	840.92	J/mol×K	1086.67	Joback Method
cpg	847.44	J/mol×K	1127.16	Joback Method
cpg	852.62	J/mol×K	1167.66	Joback Method
cpg	856.49	J/mol×K	1208.16	Joback Method
cpg	859.08	J/mol×K	1248.66	Joback Method

Sources

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=U416128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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