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

Inchi: InChI=1S/C23H26BrFO4/c1-2-3-4-5-6-7-14-28-22(26)17-8-10-18(11-9-17)23(27)29-16-19

InchiKey: KHRKTXXDYAXNLY-UHFFFAOYSA-N

Formula: C23H26BrFO4

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

Mol. weight [g/mol]: 465.35

Physical Properties

Property code	Value	Unit	Source
gf	-309.62	kJ/mol	Joback Method
hf	-738.78	kJ/mol	Joback Method
hfus	56.18	kJ/mol	Joback Method
hvap	97.26	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	6.463		Crippen Method
mcvol	321.560	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	1011.95	K	Joback Method
tc	1243.40	K	Joback Method
tf	644.08	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.91	J/mol×K	1011.95	Joback Method
cpg	1006.86	J/mol×K	1050.52	Joback Method
cpg	1017.50	J/mol×K	1089.10	Joback Method
cpg	1026.88	J/mol×K	1127.67	Joback Method
cpg	1035.04	J/mol×K	1166.25	Joback Method
cpg	1042.05	J/mol×K	1204.82	Joback Method
cpg	1047.95	J/mol×K	1243.40	Joback Method

Sources

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=U416070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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