Succinic acid, hept-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H22BrFO4/c1-3-4-5-6-12(2)22-16(20)9-10-17(21)23-15-8-7-13(19)11-14(15

InchiKey: ZLTVXDUMYUGWKI-UHFFFAOYSA-N

Formula: C17H22BrFO4

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 389.26

Physical Properties

Property code	Value	Unit	Source
gf	-465.36	kJ/mol	Joback Method
hf	-845.28	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.786		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
tb	842.57	K	Joback Method
tc	1051.01	K	Joback Method
tf	522.52	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.90	J/mol×K	842.57	Joback Method
cpg	764.28	J/mol×K	877.31	Joback Method
cpg	776.64	J/mol×K	912.05	Joback Method
cpg	787.99	J/mol×K	946.79	Joback Method
cpg	798.36	J/mol×K	981.53	Joback Method
cpg	807.77	J/mol×K	1016.27	Joback Method
cpg	816.24	J/mol×K	1051.01	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=U389768&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

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