Succinic acid, 3-methylbut-2-en-1-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C15H16BrFO4/c1-10(2)7-8-20-14(18)5-6-15(19)21-13-4-3-11(17)9-12(13)16/h

InchiKey: SIJLJMXVATXXSC-UHFFFAOYSA-N

Formula: C15H16BrFO4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 359.19

Physical Properties

Property code	Value	Unit	Source
gf	-408.09	kJ/mol	Joback Method
hf	-691.29	kJ/mol	Joback Method
hfus	40.70	kJ/mol	Joback Method
hvap	76.55	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.783		Crippen Method
mcvol	228.300	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2168.00		NIST Webbook
tb	801.29	K	Joback Method
tc	1017.65	K	Joback Method
tf	495.94	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.19	J/mol×K	801.29	Joback Method
cpg	624.42	J/mol×K	837.35	Joback Method
cpg	635.75	J/mol×K	873.41	Joback Method
cpg	646.22	J/mol×K	909.47	Joback Method
cpg	655.86	J/mol×K	945.53	Joback Method
cpg	664.70	J/mol×K	981.59	Joback Method
cpg	672.77	J/mol×K	1017.65	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=U389766&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