Succinic acid, cyclohexylmethyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H20BrFO4/c18-14-10-13(19)6-7-15(14)23-17(21)9-8-16(20)22-11-12-4-2-1

InchiKey: RCMCZHDDGVEIPF-UHFFFAOYSA-N

Formula: C17H20BrFO4

SMILES: O=C(CCC(=O)Oc1ccc(F)cc1Br)OCC1CCCCC1

Mol. weight [g/mol]: 387.24

Physical Properties

Property code	Value	Unit	Source
gf	-438.47	kJ/mol	Joback Method
hf	-785.68	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.397		Crippen Method
mcvol	249.920	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	862.56	K	Joback Method
tc	1091.12	K	Joback Method
tf	544.90	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.59	J/mol×K	862.56	Joback Method
cpg	757.66	J/mol×K	900.65	Joback Method
cpg	770.37	J/mol×K	938.75	Joback Method
cpg	781.74	J/mol×K	976.84	Joback Method
cpg	791.82	J/mol×K	1014.93	Joback Method
cpg	800.62	J/mol×K	1053.02	Joback Method
cpg	808.18	J/mol×K	1091.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389769&Units=SI
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

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