Succinic acid, 3-chlorophenyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H11BrClF3O4/c14-7-10(13(16,17)18)22-12(20)5-4-11(19)21-9-3-1-2-8(15)

InchiKey: UVNMXASQOXMWOH-UHFFFAOYSA-N

Formula: C13H11BrClF3O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 403.58

Physical Properties

Property code	Value	Unit	Source
gf	-888.12	kJ/mol	Joback Method
hf	-1167.96	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.895		Crippen Method
mcvol	220.200	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2022.00		NIST Webbook
tb	778.81	K	Joback Method
tc	990.45	K	Joback Method
tf	498.44	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.19	J/mol×K	778.81	Joback Method
cpg	583.41	J/mol×K	814.08	Joback Method
cpg	592.77	J/mol×K	849.36	Joback Method
cpg	601.31	J/mol×K	884.63	Joback Method
cpg	609.08	J/mol×K	919.90	Joback Method
cpg	616.11	J/mol×K	955.17	Joback Method
cpg	622.44	J/mol×K	990.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390830&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