Succinic acid, 1,1,1-trifluoroprop-2-yl 4-bromophenyl ester

Inchi: InChI=1S/C13H12BrF3O4/c1-8(13(15,16)17)20-11(18)6-7-12(19)21-10-4-2-9(14)3-5-10/h

InchiKey: IVBBZWKZTFQSRA-UHFFFAOYSA-N

Formula: C13H12BrF3O4

SMILES: CC(OC(=O)CCC(=O)Oc1ccc(Br)cc1)C(F)(F)F

Mol. weight [g/mol]: 369.13

Physical Properties

Property code	Value	Unit	Source
gf	-876.19	kJ/mol	Joback Method
hf	-1152.22	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.629		Crippen Method
mcvol	207.960	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	741.38	K	Joback Method
tc	949.58	K	Joback Method
tf	468.52	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.00	J/mol×K	741.38	Joback Method
cpg	562.29	J/mol×K	776.08	Joback Method
cpg	572.71	J/mol×K	810.78	Joback Method
cpg	582.30	J/mol×K	845.48	Joback Method
cpg	591.09	J/mol×K	880.18	Joback Method
cpg	599.11	J/mol×K	914.88	Joback Method
cpg	606.40	J/mol×K	949.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389816&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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