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

Inchi: InChI=1S/C13H10BrCl2F3O4/c14-7-6-9(13(17,18)19)23-11(21)5-4-10(20)22-8-3-1-2-7(15)

InchiKey: WLDGJVRGUKGPBW-UHFFFAOYSA-N

Formula: C13H10BrCl2F3O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 438.02

Physical Properties

Property code	Value	Unit	Source
gf	-909.68	kJ/mol	Joback Method
hf	-1195.17	kJ/mol	Joback Method
hfus	40.24	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.548		Crippen Method
mcvol	232.440	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	821.22	K	Joback Method
tc	1037.10	K	Joback Method
tf	540.88	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.93	J/mol×K	821.22	Joback Method
cpg	601.01	J/mol×K	857.20	Joback Method
cpg	609.26	J/mol×K	893.18	Joback Method
cpg	616.73	J/mol×K	929.16	Joback Method
cpg	623.45	J/mol×K	965.14	Joback Method
cpg	629.45	J/mol×K	1001.12	Joback Method
cpg	634.77	J/mol×K	1037.10	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=U390833&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