Succinic acid, 4-chloro-3-methylphenyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C14H13BrClF3O4/c1-8-6-9(2-3-10(8)16)22-12(20)4-5-13(21)23-11(7-15)14(17

InchiKey: VDLPSOBOTMTZAS-UHFFFAOYSA-N

Formula: C14H13BrClF3O4

SMILES: Cc1cc(OC(=O)CCC(=O)OC(CBr)C(F)(F)F)ccc1Cl

Mol. weight [g/mol]: 417.60

Physical Properties

Property code	Value	Unit	Source
gf	-889.33	kJ/mol	Joback Method
hf	-1200.07	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.203		Crippen Method
mcvol	234.290	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	806.67	K	Joback Method
tc	1017.28	K	Joback Method
tf	522.23	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.78	J/mol×K	806.67	Joback Method
cpg	635.32	J/mol×K	841.77	Joback Method
cpg	644.99	J/mol×K	876.87	Joback Method
cpg	653.84	J/mol×K	911.98	Joback Method
cpg	661.89	J/mol×K	947.08	Joback Method
cpg	669.17	J/mol×K	982.18	Joback Method
cpg	675.73	J/mol×K	1017.28	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=U390832&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

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