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

Inchi: InChI=1S/C14H20BrF3O4/c15-8-11(14(16,17)18)22-13(20)7-6-12(19)21-9-10-4-2-1-3-5-1

InchiKey: PDUADIKPVNPHLG-UHFFFAOYSA-N

Formula: C14H20BrF3O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)OCC1CCCCC1

Mol. weight [g/mol]: 389.20

Physical Properties

Property code	Value	Unit	Source
gf	-946.10	kJ/mol	Joback Method
hf	-1343.60	kJ/mol	Joback Method
hfus	33.01	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.759		Crippen Method
mcvol	234.950	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	752.15	K	Joback Method
tc	952.75	K	Joback Method
tf	448.23	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.09	J/mol×K	752.15	Joback Method
cpg	702.04	J/mol×K	785.58	Joback Method
cpg	715.92	J/mol×K	819.02	Joback Method
cpg	728.76	J/mol×K	852.45	Joback Method
cpg	740.61	J/mol×K	885.89	Joback Method
cpg	751.49	J/mol×K	919.32	Joback Method
cpg	761.45	J/mol×K	952.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390828&Units=SI

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