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

Inchi: InChI=1S/C9H10BrCl2F3O4/c10-3-5(9(13,14)15)19-8(17)2-1-7(16)18-4-6(11)12/h5-6H,1

InchiKey: XIOUTOGAFJPRCP-UHFFFAOYSA-N

Formula: C9H10BrCl2F3O4

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

Mol. weight [g/mol]: 389.98

Physical Properties

Property code	Value	Unit	Source
gf	-1038.95	kJ/mol	Joback Method
hf	-1331.48	kJ/mol	Joback Method
hfus	33.10	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.982		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	692.62	K	Joback Method
tc	887.26	K	Joback Method
tf	429.34	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.99	J/mol×K	692.62	Joback Method
cpg	492.39	J/mol×K	725.06	Joback Method
cpg	501.15	J/mol×K	757.50	Joback Method
cpg	509.27	J/mol×K	789.94	Joback Method
cpg	516.78	J/mol×K	822.38	Joback Method
cpg	523.70	J/mol×K	854.82	Joback Method
cpg	530.05	J/mol×K	887.26	Joback Method

Sources

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=U390823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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