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

Inchi: InChI=1S/C10H10BrF7O4/c11-3-5(10(16,17)18)22-7(20)2-1-6(19)21-4-9(14,15)8(12)13/h

InchiKey: GCAVVOHOOSFGRX-UHFFFAOYSA-N

Formula: C10H10BrF7O4

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

Mol. weight [g/mol]: 407.08

Physical Properties

Property code	Value	Unit	Source
gf	-1783.07	kJ/mol	Joback Method
hf	-2113.83	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.079		Crippen Method
mcvol	196.530	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1381.00		NIST Webbook
tb	634.49	K	Joback Method
tc	801.96	K	Joback Method
tf	385.55	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.52	J/mol×K	634.49	Joback Method
cpg	530.83	J/mol×K	662.40	Joback Method
cpg	540.51	J/mol×K	690.31	Joback Method
cpg	549.58	J/mol×K	718.22	Joback Method
cpg	558.07	J/mol×K	746.14	Joback Method
cpg	566.00	J/mol×K	774.05	Joback Method
cpg	573.40	J/mol×K	801.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390819&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

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