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

Inchi: InChI=1S/C10H11BrF6O4/c1-5(9(12,13)14)20-7(18)2-3-8(19)21-6(4-11)10(15,16)17/h5-6

InchiKey: PEJWYSLJAQCNSK-UHFFFAOYSA-N

Formula: C10H11BrF6O4

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

Mol. weight [g/mol]: 389.09

Physical Properties

Property code	Value	Unit	Source
gf	-1588.26	kJ/mol	Joback Method
hf	-1917.72	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.130		Crippen Method
mcvol	194.760	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
tb	635.22	K	Joback Method
tc	808.34	K	Joback Method
tf	384.96	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.40	J/mol×K	635.22	Joback Method
cpg	523.11	J/mol×K	664.07	Joback Method
cpg	533.14	J/mol×K	692.93	Joback Method
cpg	542.54	J/mol×K	721.78	Joback Method
cpg	551.33	J/mol×K	750.64	Joback Method
cpg	559.52	J/mol×K	779.49	Joback Method
cpg	567.17	J/mol×K	808.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390818&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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