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

Inchi: InChI=1S/C9H12BrF3O4/c1-2-16-7(14)3-4-8(15)17-6(5-10)9(11,12)13/h6H,2-5H2,1H3
InchiKey: FHYCJGWPEZMKPJ-UHFFFAOYSA-N
Formula: C9H12BrF3O4
SMILES: CCOC(=O)CCC(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 321.09

Physical Properties

Property code	Value	Unit	Source
gf	-1012.65	kJ/mol	Joback Method
hf	-1294.72	kJ/mol	Joback Method
hfus	28.23	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.199		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1358.00		NIST Webbook
tb	618.20	K	Joback Method
tc	801.58	K	Joback Method
tf	384.50	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.35	J/mol×K	618.20	Joback Method
cpg	446.19	J/mol×K	648.76	Joback Method
cpg	456.42	J/mol×K	679.33	Joback Method
cpg	466.06	J/mol×K	709.89	Joback Method
cpg	475.12	J/mol×K	740.46	Joback Method
cpg	483.62	J/mol×K	771.02	Joback Method
cpg	491.57	J/mol×K	801.58	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=U390839&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