Succinic acid, 8-chlorooctyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H23BrClF3O4/c16-11-12(15(18,19)20)24-14(22)8-7-13(21)23-10-6-4-2-1-3

InchiKey: GZOGOKOEMUQTEV-UHFFFAOYSA-N

Formula: C15H23BrClF3O4

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

Mol. weight [g/mol]: 439.69

Physical Properties

Property code	Value	Unit	Source
gf	-974.06	kJ/mol	Joback Method
hf	-1434.30	kJ/mol	Joback Method
hfus	47.96	kJ/mol	Joback Method
hvap	73.98	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.758		Crippen Method
mcvol	272.140	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	792.91	K	Joback Method
tc	979.37	K	Joback Method
tf	482.04	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.19	J/mol×K	792.91	Joback Method
cpg	789.28	J/mol×K	823.99	Joback Method
cpg	801.55	J/mol×K	855.06	Joback Method
cpg	813.02	J/mol×K	886.14	Joback Method
cpg	823.74	J/mol×K	917.21	Joback Method
cpg	833.72	J/mol×K	948.29	Joback Method
cpg	843.00	J/mol×K	979.37	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=U390834&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