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

Inchi: InChI=1S/C17H28BrF3O4/c1-3-4-5-6-7-8-9-13(2)24-15(22)10-11-16(23)25-14(12-18)17(

InchiKey: KQNBOZGQZUYGOF-UHFFFAOYSA-N

Formula: C17H28BrF3O4

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

Mol. weight [g/mol]: 433.30

Physical Properties

Property code	Value	Unit	Source
gf	-947.73	kJ/mol	Joback Method
hf	-1465.12	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.318		Crippen Method
mcvol	288.080	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	800.80	K	Joback Method
tc	986.25	K	Joback Method
tf	459.66	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.27	J/mol×K	800.80	Joback Method
cpg	878.19	J/mol×K	831.71	Joback Method
cpg	892.19	J/mol×K	862.62	Joback Method
cpg	905.32	J/mol×K	893.53	Joback Method
cpg	917.59	J/mol×K	924.44	Joback Method
cpg	929.05	J/mol×K	955.34	Joback Method
cpg	939.73	J/mol×K	986.25	Joback Method

Sources

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=U390831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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