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

Inchi: InChI=1S/C15H24BrF3O4/c1-3-5-6-11(4-2)10-22-13(20)7-8-14(21)23-12(9-16)15(17,18)

InchiKey: NRGYBVLCZJZXOP-UHFFFAOYSA-N

Formula: C15H24BrF3O4

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

Mol. weight [g/mol]: 405.25

Physical Properties

Property code	Value	Unit	Source
gf	-964.57	kJ/mol	Joback Method
hf	-1423.84	kJ/mol	Joback Method
hfus	40.24	kJ/mol	Joback Method
hvap	69.21	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.395		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	755.04	K	Joback Method
tc	937.62	K	Joback Method
tf	437.12	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.57	J/mol×K	755.04	Joback Method
cpg	763.69	J/mol×K	785.47	Joback Method
cpg	776.97	J/mol×K	815.90	Joback Method
cpg	789.44	J/mol×K	846.33	Joback Method
cpg	801.13	J/mol×K	876.76	Joback Method
cpg	812.07	J/mol×K	907.19	Joback Method
cpg	822.28	J/mol×K	937.62	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=U390827&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