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

Inchi: InChI=1S/C20H30BrF3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-27-18(25)13-14-19(26)28-17(

InchiKey: RQLHKFVRZOOXKV-UHFFFAOYSA-N

Formula: C20H30BrF3O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 471.35

Physical Properties

Property code	Value	Unit	Source
gf	-717.23	kJ/mol	Joback Method
hf	-1249.46	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.713		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	878.88	K	Joback Method
tc	1078.04	K	Joback Method
tf	614.57	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.23	J/mol×K	878.88	Joback Method
cpg	1002.28	J/mol×K	912.07	Joback Method
cpg	1016.31	J/mol×K	945.27	Joback Method
cpg	1029.37	J/mol×K	978.46	Joback Method
cpg	1041.51	J/mol×K	1011.66	Joback Method
cpg	1052.77	J/mol×K	1044.85	Joback Method
cpg	1063.19	J/mol×K	1078.04	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=U390836&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