Succinic acid, naphth-2-ylmethyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C18H16BrF3O4/c19-10-15(18(20,21)22)26-17(24)8-7-16(23)25-11-12-5-6-13-3

InchiKey: UZKUQCUGTQSKPW-UHFFFAOYSA-N

Formula: C18H16BrF3O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 433.22

Physical Properties

Property code	Value	Unit	Source
gf	-727.44	kJ/mol	Joback Method
hf	-1064.35	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	80.85	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.532		Crippen Method
mcvol	258.950	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2641.00		NIST Webbook
rinpol	2641.00		NIST Webbook
tb	874.76	K	Joback Method
tc	1092.63	K	Joback Method
tf	557.57	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.39	J/mol×K	874.76	Joback Method
cpg	758.72	J/mol×K	911.07	Joback Method
cpg	769.17	J/mol×K	947.38	Joback Method
cpg	778.84	J/mol×K	983.69	Joback Method
cpg	787.80	J/mol×K	1020.01	Joback Method
cpg	796.13	J/mol×K	1056.32	Joback Method
cpg	803.92	J/mol×K	1092.63	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=U390837&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