Succinic acid, naphth-2-ylmethyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C19H16F6O4/c20-17(19(23,24)25)18(21,22)11-29-16(27)8-7-15(26)28-10-12-5

InchiKey: XMZFDZHTPKKLRV-UHFFFAOYSA-N

Formula: C19H16F6O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)C(F)(F)F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 422.32

Physical Properties

Property code	Value	Unit	Source
gf	-1314.93	kJ/mol	Joback Method
hf	-1708.40	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.742		Crippen Method
mcvol	260.850	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	826.06	K	Joback Method
tc	1024.02	K	Joback Method
tf	513.23	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.77	J/mol×K	826.06	Joback Method
cpg	805.79	J/mol×K	859.05	Joback Method
cpg	816.94	J/mol×K	892.05	Joback Method
cpg	827.27	J/mol×K	925.04	Joback Method
cpg	836.87	J/mol×K	958.03	Joback Method
cpg	845.82	J/mol×K	991.02	Joback Method
cpg	854.17	J/mol×K	1024.02	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=U390816&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