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

Inchi: InChI=1S/C20H18F6O4/c21-18(20(24,25)26)19(22,23)12-30-17(28)7-3-6-16(27)29-11-13

InchiKey: KNQHWAHMXAGPMD-UHFFFAOYSA-N

Formula: C20H18F6O4

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

Mol. weight [g/mol]: 436.34

Physical Properties

Property code	Value	Unit	Source
gf	-1306.51	kJ/mol	Joback Method
hf	-1729.04	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	75.12	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.132		Crippen Method
mcvol	274.940	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	848.94	K	Joback Method
tc	1047.90	K	Joback Method
tf	524.50	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.02	J/mol×K	848.94	Joback Method
cpg	862.39	J/mol×K	882.10	Joback Method
cpg	873.88	J/mol×K	915.26	Joback Method
cpg	884.56	J/mol×K	948.42	Joback Method
cpg	894.50	J/mol×K	981.58	Joback Method
cpg	903.79	J/mol×K	1014.74	Joback Method
cpg	912.50	J/mol×K	1047.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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