Glutaric acid, naphth-2-ylmethyl pentafluorobenzyl ester

Inchi: InChI=1S/C23H17F5O4/c24-19-16(20(25)22(27)23(28)21(19)26)12-32-18(30)7-3-6-17(29

InchiKey: ULALZRLFPGPQBB-UHFFFAOYSA-N

Formula: C23H17F5O4

SMILES: O=C(CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 452.37

Physical Properties

Property code	Value	Unit	Source
gf	-1025.42	kJ/mol	Joback Method
hf	-1392.89	kJ/mol	Joback Method
hfus	59.07	kJ/mol	Joback Method
hvap	91.18	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	5.492		Crippen Method
mcvol	291.680	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	976.79	K	Joback Method
tc	1197.85	K	Joback Method
tf	656.90	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.29	J/mol×K	976.79	Joback Method
cpg	914.11	J/mol×K	1013.63	Joback Method
cpg	923.83	J/mol×K	1050.48	Joback Method
cpg	932.50	J/mol×K	1087.32	Joback Method
cpg	940.16	J/mol×K	1124.16	Joback Method
cpg	946.85	J/mol×K	1161.01	Joback Method
cpg	952.62	J/mol×K	1197.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391945&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

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