Glutaric acid, naphth-2-ylmethyl 2-fluoroethyl ester

Inchi: InChI=1S/C18H19FO4/c19-10-11-22-17(20)6-3-7-18(21)23-13-14-8-9-15-4-1-2-5-16(15)1

InchiKey: WHKFGRRUPFPHHN-UHFFFAOYSA-N

Formula: C18H19FO4

SMILES: O=C(CCCC(=O)OCc1ccc2ccccc2c1)OCCF

Mol. weight [g/mol]: 318.34

Physical Properties

Property code	Value	Unit	Source
gf	-352.54	kJ/mol	Joback Method
hf	-684.43	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	77.73	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.566		Crippen Method
mcvol	237.910	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2583.00		NIST Webbook
rinpol	2583.00		NIST Webbook
tb	813.73	K	Joback Method
tc	1023.72	K	Joback Method
tf	509.17	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.51	J/mol×K	813.73	Joback Method
cpg	710.02	J/mol×K	848.73	Joback Method
cpg	722.56	J/mol×K	883.73	Joback Method
cpg	734.16	J/mol×K	918.73	Joback Method
cpg	744.87	J/mol×K	953.73	Joback Method
cpg	754.73	J/mol×K	988.72	Joback Method
cpg	763.77	J/mol×K	1023.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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