Glutaric acid, (cyclohex-3-enyl)methyl 2-fluorophenyl ester

Inchi: InChI=1S/C18H21FO4/c19-15-9-4-5-10-16(15)23-18(21)12-6-11-17(20)22-13-14-7-2-1-3

InchiKey: ULZHRPSFVDEUMZ-UHFFFAOYSA-N

Formula: C18H21FO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCC1CC=CCC1

Mol. weight [g/mol]: 320.36

Physical Properties

Property code	Value	Unit	Source
gf	-404.78	kJ/mol	Joback Method
hf	-763.40	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	76.82	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.801		Crippen Method
mcvol	242.210	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	2369.00		NIST Webbook
tb	813.46	K	Joback Method
tc	1030.76	K	Joback Method
tf	484.61	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.86	J/mol×K	813.46	Joback Method
cpg	751.43	J/mol×K	849.68	Joback Method
cpg	765.68	J/mol×K	885.89	Joback Method
cpg	778.64	J/mol×K	922.11	Joback Method
cpg	790.35	J/mol×K	958.33	Joback Method
cpg	800.81	J/mol×K	994.54	Joback Method
cpg	810.07	J/mol×K	1030.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405528&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