Glutaric acid, cyclohexylmethyl 3-fluorophenyl ester

Inchi: InChI=1S/C18H23FO4/c19-15-8-4-9-16(12-15)23-18(21)11-5-10-17(20)22-13-14-6-2-1-3

InchiKey: ISSADMMOLBCSJU-UHFFFAOYSA-N

Formula: C18H23FO4

SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)OCC1CCCCC1

Mol. weight [g/mol]: 322.37

Physical Properties

Property code	Value	Unit	Source
gf	-434.74	kJ/mol	Joback Method
hf	-821.18	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.025		Crippen Method
mcvol	246.510	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	814.30	K	Joback Method
tc	1030.28	K	Joback Method
tf	483.85	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.35	J/mol×K	814.30	Joback Method
cpg	779.74	J/mol×K	850.30	Joback Method
cpg	794.77	J/mol×K	886.29	Joback Method
cpg	808.46	J/mol×K	922.29	Joback Method
cpg	820.84	J/mol×K	958.29	Joback Method
cpg	831.94	J/mol×K	994.28	Joback Method
cpg	841.78	J/mol×K	1030.28	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=U392093&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