Glutaric acid, 3,5-difluorophenyl pentyl ester

Inchi: InChI=1S/C16H20F2O4/c1-2-3-4-8-21-15(19)6-5-7-16(20)22-14-10-12(17)9-13(18)11-14
InchiKey: IWNUMCGJVWCQKW-UHFFFAOYSA-N
Formula: C16H20F2O4
SMILES: CCCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 314.32

Physical Properties

Property code	Value	Unit	Source
gf	-680.47	kJ/mol	Joback Method
hf	-1041.80	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.774		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	753.24	K	Joback Method
tc	943.80	K	Joback Method
tf	467.04	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.08	J/mol×K	753.24	Joback Method
cpg	677.05	J/mol×K	785.00	Joback Method
cpg	690.16	J/mol×K	816.76	Joback Method
cpg	702.41	J/mol×K	848.52	Joback Method
cpg	713.82	J/mol×K	880.28	Joback Method
cpg	724.40	J/mol×K	912.04	Joback Method
cpg	734.14	J/mol×K	943.80	Joback Method

Sources

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=U358629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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