Glutaric acid, 3,5-difluorophenyl hexyl ester

Inchi: InChI=1S/C17H22F2O4/c1-2-3-4-5-9-22-16(20)7-6-8-17(21)23-15-11-13(18)10-14(19)12
InchiKey: QGMRRAGDPZYERA-UHFFFAOYSA-N
Formula: C17H22F2O4
SMILES: CCCCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-672.05	kJ/mol	Joback Method
hf	-1062.44	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.164		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	776.12	K	Joback Method
tc	966.64	K	Joback Method
tf	478.31	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.85	J/mol×K	776.12	Joback Method
cpg	733.19	J/mol×K	807.87	Joback Method
cpg	746.62	J/mol×K	839.63	Joback Method
cpg	759.15	J/mol×K	871.38	Joback Method
cpg	770.80	J/mol×K	903.13	Joback Method
cpg	781.57	J/mol×K	934.89	Joback Method
cpg	791.47	J/mol×K	966.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358631&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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