Glutaric acid, 3-fluorophenyl octyl ester

Inchi: InChI=1S/C19H27FO4/c1-2-3-4-5-6-7-14-23-18(21)12-9-13-19(22)24-17-11-8-10-16(20)1
InchiKey: XTLXAAPAMQUMCA-UHFFFAOYSA-N
Formula: C19H27FO4
SMILES: CCCCCCCCOC(=O)CCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-450.77	kJ/mol	Joback Method
hf	-896.14	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.805		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2408.00		NIST Webbook
tb	817.63	K	Joback Method
tc	1012.75	K	Joback Method
tf	487.74	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.52	J/mol×K	817.63	Joback Method
cpg	841.99	J/mol×K	850.15	Joback Method
cpg	856.41	J/mol×K	882.67	Joback Method
cpg	869.82	J/mol×K	915.19	Joback Method
cpg	882.22	J/mol×K	947.71	Joback Method
cpg	893.63	J/mol×K	980.23	Joback Method
cpg	904.08	J/mol×K	1012.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359052&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

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