Glutaric acid, 8-chlorooctyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C20H28ClFO5/c1-25-18-15-16(22)11-12-17(18)27-20(24)10-8-9-19(23)26-14-7

InchiKey: SPHATFVBNJENNK-UHFFFAOYSA-N

Formula: C20H28ClFO5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 402.88

Physical Properties

Property code	Value	Unit	Source
gf	-568.91	kJ/mol	Joback Method
hf	-1076.21	kJ/mol	Joback Method
hfus	54.86	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.033		Crippen Method
mcvol	303.660	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook
tb	905.34	K	Joback Method
tc	1111.14	K	Joback Method
tf	563.68	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.71	J/mol×K	905.34	Joback Method
cpg	953.75	J/mol×K	939.64	Joback Method
cpg	966.53	J/mol×K	973.94	Joback Method
cpg	978.08	J/mol×K	1008.24	Joback Method
cpg	988.40	J/mol×K	1042.54	Joback Method
cpg	997.50	J/mol×K	1076.84	Joback Method
cpg	1005.38	J/mol×K	1111.14	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=U393451&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