Glutaric acid, 2-chloro-6-fluorophenyl pentadecyl ester

Inchi: InChI=1S/C26H40ClFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-31-24(29)19-16-20-25(30

InchiKey: GNOJNTRUXSJBNM-UHFFFAOYSA-N

Formula: C26H40ClFO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 471.05

Physical Properties

Property code	Value	Unit	Source
gf	-413.39	kJ/mol	Joback Method
hf	-1067.83	kJ/mol	Joback Method
hfus	69.21	kJ/mol	Joback Method
hvap	98.95	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.189		Crippen Method
mcvol	382.330	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		NIST Webbook
tb	1020.20	K	Joback Method
tc	1253.10	K	Joback Method
tf	609.07	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.61	J/mol×K	1020.20	Joback Method
cpg	1291.87	J/mol×K	1059.02	Joback Method
cpg	1306.47	J/mol×K	1097.83	Joback Method
cpg	1319.45	J/mol×K	1136.65	Joback Method
cpg	1330.87	J/mol×K	1175.46	Joback Method
cpg	1340.79	J/mol×K	1214.28	Joback Method
cpg	1349.27	J/mol×K	1253.10	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=U391657&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