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

Inchi: InChI=1S/C24H36ClFO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-29-22(27)17-14-18-23(28)30-24
InchiKey: RQFCCOFHSLFAQD-UHFFFAOYSA-N
Formula: C24H36ClFO4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 442.99

Physical Properties

Property code	Value	Unit	Source
gf	-430.23	kJ/mol	Joback Method
hf	-1026.55	kJ/mol	Joback Method
hfus	64.03	kJ/mol	Joback Method
hvap	94.50	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.409		Crippen Method
mcvol	354.150	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	974.44	K	Joback Method
tc	1193.27	K	Joback Method
tf	586.53	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.18	J/mol×K	974.44	Joback Method
cpg	1167.81	J/mol×K	1010.91	Joback Method
cpg	1182.00	J/mol×K	1047.38	Joback Method
cpg	1194.80	J/mol×K	1083.85	Joback Method
cpg	1206.23	J/mol×K	1120.32	Joback Method
cpg	1216.35	J/mol×K	1156.80	Joback Method
cpg	1225.18	J/mol×K	1193.27	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=U391630&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

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