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

Inchi: InChI=1S/C16H18ClFO4/c17-12-7-3-8-13(18)16(12)22-15(20)10-4-9-14(19)21-11-5-1-2-(

InchiKey: ZCQMHHJPJQABIR-UHFFFAOYSA-N

Formula: C16H18ClFO4

SMILES: O=C(CCCC(=O)OC1CCCC1)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 328.76

Physical Properties

Property code	Value	Unit	Source
gf	-461.04	kJ/mol	Joback Method
hf	-800.95	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	76.95	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.041		Crippen Method
mcvol	230.570	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
tb	806.68	K	Joback Method
tc	1026.03	K	Joback Method
tf	507.27	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.61	J/mol×K	806.68	Joback Method
cpg	685.86	J/mol×K	843.24	Joback Method
cpg	698.93	J/mol×K	879.80	Joback Method
cpg	710.84	J/mol×K	916.35	Joback Method
cpg	721.61	J/mol×K	952.91	Joback Method
cpg	731.27	J/mol×K	989.47	Joback Method
cpg	739.85	J/mol×K	1026.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405396&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