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

Inchi: InChI=1S/C18H22ClFO4/c19-14-8-4-9-15(20)18(14)24-17(22)11-5-10-16(21)23-12-13-6-

InchiKey: VNKINHSWHPUMBS-UHFFFAOYSA-N

Formula: C18H22ClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCC1CCCCC1

Mol. weight [g/mol]: 356.82

Physical Properties

Property code	Value	Unit	Source
gf	-456.30	kJ/mol	Joback Method
hf	-848.39	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.678		Crippen Method
mcvol	258.750	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	856.71	K	Joback Method
tc	1076.96	K	Joback Method
tf	526.29	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.79	J/mol×K	856.71	Joback Method
cpg	803.58	J/mol×K	893.42	Joback Method
cpg	816.99	J/mol×K	930.13	Joback Method
cpg	829.06	J/mol×K	966.83	Joback Method
cpg	839.79	J/mol×K	1003.54	Joback Method
cpg	849.22	J/mol×K	1040.25	Joback Method
cpg	857.37	J/mol×K	1076.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391586&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/118-156-8/Glutaric-acid-cyclohexylmethyl-2-chloro-6-fluorophenyl-ester.pdf
Generated by Cheméo on 2024-04-27 05:58:48.659936503 +0000 UTC m=+16486777.580513818.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.