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

Inchi: InChI=1S/C18H20ClFO4/c19-13-3-1-4-14(20)18(13)24-17(22)6-2-5-16(21)23-15-10-11-7

InchiKey: ZVPJPUJXGKQTCW-UHFFFAOYSA-N

Formula: C18H20ClFO4

SMILES: O=C(CCCC(=O)OC1CC2CCC1C2)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 354.80

Physical Properties

Property code	Value	Unit	Source
gf	-379.06	kJ/mol	Joback Method
hf	-783.61	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.287		Crippen Method
mcvol	247.890	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	850.24	K	Joback Method
tc	1070.62	K	Joback Method
tf	547.03	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.31	J/mol×K	850.24	Joback Method
cpg	783.07	J/mol×K	886.97	Joback Method
cpg	796.70	J/mol×K	923.70	Joback Method
cpg	809.26	J/mol×K	960.43	Joback Method
cpg	820.80	J/mol×K	997.16	Joback Method
cpg	831.40	J/mol×K	1033.89	Joback Method
cpg	841.10	J/mol×K	1070.62	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=U405495&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