Glutaric acid, hex-4-yn-3-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H18ClFO4/c1-3-7-12(4-2)22-15(20)10-6-11-16(21)23-17-13(18)8-5-9-14(1
InchiKey: INTXJVAMMLJPOG-UHFFFAOYSA-N
Formula: C17H18ClFO4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 340.77

Physical Properties

Property code	Value	Unit	Source
gf	-288.81	kJ/mol	Joback Method
hf	-615.05	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.900		Crippen Method
mcvol	246.920	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	822.84	K	Joback Method
tc	1039.81	K	Joback Method
tf	598.74	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.21	J/mol×K	822.84	Joback Method
cpg	700.35	J/mol×K	859.00	Joback Method
cpg	712.43	J/mol×K	895.16	Joback Method
cpg	723.46	J/mol×K	931.33	Joback Method
cpg	733.46	J/mol×K	967.49	Joback Method
cpg	742.42	J/mol×K	1003.65	Joback Method
cpg	750.37	J/mol×K	1039.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391583&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