Glutaric acid, 2-chloro-6-fluorophenyl non-5-yn-3-yl ester

Inchi: InChI=1S/C20H24ClFO4/c1-3-5-6-7-10-15(4-2)25-18(23)13-9-14-19(24)26-20-16(21)11-8

InchiKey: MOKWDUDXVLGGRL-UHFFFAOYSA-N

Formula: C20H24ClFO4

SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 382.85

Physical Properties

Property code	Value	Unit	Source
gf	-263.55	kJ/mol	Joback Method
hf	-676.97	kJ/mol	Joback Method
hfus	53.27	kJ/mol	Joback Method
hvap	87.36	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.070		Crippen Method
mcvol	289.190	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	891.48	K	Joback Method
tc	1105.76	K	Joback Method
tf	632.55	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.18	J/mol×K	891.48	Joback Method
cpg	871.93	J/mol×K	927.19	Joback Method
cpg	884.50	J/mol×K	962.91	Joback Method
cpg	895.92	J/mol×K	998.62	Joback Method
cpg	906.19	J/mol×K	1034.33	Joback Method
cpg	915.35	J/mol×K	1070.04	Joback Method
cpg	923.41	J/mol×K	1105.76	Joback Method

Sources

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=U393956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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