Glutaric acid, hex-4-yn-3-yl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C18H21ClO4/c1-4-7-14(5-2)22-17(20)8-6-9-18(21)23-16-12-13(3)10-11-15(16)

InchiKey: UQFQSCZAHCIIRW-UHFFFAOYSA-N

Formula: C18H21ClO4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 336.81

Physical Properties

Property code	Value	Unit	Source
gf	-85.58	kJ/mol	Joback Method
hf	-439.58	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	83.72	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.069		Crippen Method
mcvol	259.240	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2386.00		NIST Webbook
rinpol	2386.00		NIST Webbook
tb	846.45	K	Joback Method
tc	1068.37	K	Joback Method
tf	609.42	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.95	J/mol×K	846.45	Joback Method
cpg	749.83	J/mol×K	883.44	Joback Method
cpg	762.56	J/mol×K	920.42	Joback Method
cpg	774.15	J/mol×K	957.41	Joback Method
cpg	784.60	J/mol×K	994.40	Joback Method
cpg	793.93	J/mol×K	1031.38	Joback Method
cpg	802.15	J/mol×K	1068.37	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=U393421&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