Glutaric acid, hex-4-yn-3-yl 3-chlorophenyl ester

Inchi: InChI=1S/C17H19ClO4/c1-3-7-14(4-2)21-16(19)10-6-11-17(20)22-15-9-5-8-13(18)12-15/

InchiKey: CGYSEEPURQNZRH-UHFFFAOYSA-N

Formula: C17H19ClO4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 322.78

Physical Properties

Property code	Value	Unit	Source
gf	-84.37	kJ/mol	Joback Method
hf	-407.47	kJ/mol	Joback Method
hfus	42.81	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.761		Crippen Method
mcvol	245.150	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	818.59	K	Joback Method
tc	1042.06	K	Joback Method
tf	585.63	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.91	J/mol×K	818.59	Joback Method
cpg	694.68	J/mol×K	855.84	Joback Method
cpg	707.33	J/mol×K	893.08	Joback Method
cpg	718.87	J/mol×K	930.33	Joback Method
cpg	729.31	J/mol×K	967.57	Joback Method
cpg	738.69	J/mol×K	1004.82	Joback Method
cpg	747.00	J/mol×K	1042.06	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=U390461&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