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

Inchi: InChI=1S/C18H21ClO5/c1-4-7-14(5-2)23-17(20)8-6-9-18(21)24-15-11-10-13(19)12-16(15

InchiKey: QYYBGDFXPFOCHM-UHFFFAOYSA-N

Formula: C18H21ClO5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 352.81

Physical Properties

Property code	Value	Unit	Source
gf	-190.58	kJ/mol	Joback Method
hf	-571.80	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.769		Crippen Method
mcvol	265.110	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	868.87	K	Joback Method
tc	1089.82	K	Joback Method
tf	631.65	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.94	J/mol×K	868.87	Joback Method
cpg	776.23	J/mol×K	905.69	Joback Method
cpg	788.27	J/mol×K	942.52	Joback Method
cpg	799.07	J/mol×K	979.34	Joback Method
cpg	808.62	J/mol×K	1016.17	Joback Method
cpg	816.91	J/mol×K	1052.99	Joback Method
cpg	823.94	J/mol×K	1089.82	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=U393907&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