Glutaric acid, but-3-yn-2-yl 4-chlorobenzyl ester

Inchi: InChI=1S/C16H17ClO4/c1-3-12(2)21-16(19)6-4-5-15(18)20-11-13-7-9-14(17)10-8-13/h1,
InchiKey: YIZRZEGAZRSTFD-UHFFFAOYSA-N
Formula: C16H17ClO4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 308.76

Physical Properties

Property code	Value	Unit	Source
gf	-72.52	kJ/mol	Joback Method
hf	-367.23	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.118		Crippen Method
mcvol	231.060	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	776.83	K	Joback Method
tc	995.13	K	Joback Method
tf	515.23	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.43	J/mol×K	776.83	Joback Method
cpg	636.68	J/mol×K	813.21	Joback Method
cpg	648.92	J/mol×K	849.60	Joback Method
cpg	660.18	J/mol×K	885.98	Joback Method
cpg	670.48	J/mol×K	922.36	Joback Method
cpg	679.86	J/mol×K	958.75	Joback Method
cpg	688.32	J/mol×K	995.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391723&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