Glutaric acid, hex-4-yn-3-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C19H24O5/c1-5-8-15(6-2)23-18(20)9-7-10-19(21)24-17-13-14(3)11-12-16(17)2

InchiKey: CNSIDOXHBQSTNA-UHFFFAOYSA-N

Formula: C19H24O5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	-170.23	kJ/mol	Joback Method
hf	-576.70	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.424		Crippen Method
mcvol	266.960	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	854.32	K	Joback Method
tc	1070.23	K	Joback Method
tf	613.00	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.91	J/mol×K	854.32	Joback Method
cpg	810.67	J/mol×K	890.31	Joback Method
cpg	824.17	J/mol×K	926.29	Joback Method
cpg	836.42	J/mol×K	962.28	Joback Method
cpg	847.41	J/mol×K	998.26	Joback Method
cpg	857.13	J/mol×K	1034.25	Joback Method
cpg	865.59	J/mol×K	1070.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393924&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

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