Glutaric acid, tridec-2-yn-1-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C26H38O5/c1-4-5-6-7-8-9-10-11-12-13-14-20-30-25(27)16-15-17-26(28)31-24

InchiKey: VRUPUOLJFYFORP-UHFFFAOYSA-N

Formula: C26H38O5

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 430.58

Physical Properties

Property code	Value	Unit	Source
gf	-108.85	kJ/mol	Joback Method
hf	-715.90	kJ/mol	Joback Method
hfus	66.24	kJ/mol	Joback Method
hvap	99.94	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.157		Crippen Method
mcvol	365.590	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	3186.00		NIST Webbook
tb	1014.92	K	Joback Method
tc	1242.56	K	Joback Method
tf	706.89	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1214.95	J/mol×K	1014.92	Joback Method
cpg	1230.13	J/mol×K	1052.86	Joback Method
cpg	1243.57	J/mol×K	1090.80	Joback Method
cpg	1255.30	J/mol×K	1128.74	Joback Method
cpg	1265.34	J/mol×K	1166.68	Joback Method
cpg	1273.72	J/mol×K	1204.62	Joback Method
cpg	1280.45	J/mol×K	1242.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393934&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