Glutaric acid, tridec-2-yn-1-yl 4-acetylphenyl ester

Inchi: InChI=1S/C26H36O5/c1-3-4-5-6-7-8-9-10-11-12-13-21-30-25(28)15-14-16-26(29)31-24-1

InchiKey: LOTWSRXGDZTQKA-UHFFFAOYSA-N

Formula: C26H36O5

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 428.56

Physical Properties

Property code	Value	Unit	Source
gf	-123.14	kJ/mol	Joback Method
hf	-684.79	kJ/mol	Joback Method
hfus	67.04	kJ/mol	Joback Method
hvap	103.62	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.042		Crippen Method
mcvol	361.290	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	3346.00		NIST Webbook
rinpol	3346.00		NIST Webbook
tb	1041.39	K	Joback Method
tc	1274.98	K	Joback Method
tf	722.07	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.88	J/mol×K	1041.39	Joback Method
cpg	1213.00	J/mol×K	1080.32	Joback Method
cpg	1225.52	J/mol×K	1119.25	Joback Method
cpg	1236.50	J/mol×K	1158.19	Joback Method
cpg	1245.97	J/mol×K	1197.12	Joback Method
cpg	1254.00	J/mol×K	1236.05	Joback Method
cpg	1260.62	J/mol×K	1274.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392040&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