Glutaric acid, hex-4-yn-3-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H26O5/c1-3-10-20(4-2)29-24(26)16-9-15-23(25)27-18-19-11-8-14-22(17-1

InchiKey: SBYGSDUIILINPF-UHFFFAOYSA-N

Formula: C24H26O5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 394.46

Physical Properties

Property code	Value	Unit	Source
gf	-6.09	kJ/mol	Joback Method
hf	-431.90	kJ/mol	Joback Method
hfus	51.97	kJ/mol	Joback Method
hvap	96.72	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.037		Crippen Method
mcvol	313.650	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2968.00		NIST Webbook
tb	990.42	K	Joback Method
tc	1226.48	K	Joback Method
tf	683.25	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.16	J/mol×K	990.42	Joback Method
cpg	999.76	J/mol×K	1029.76	Joback Method
cpg	1010.75	J/mol×K	1069.11	Joback Method
cpg	1020.17	J/mol×K	1108.45	Joback Method
cpg	1028.05	J/mol×K	1147.79	Joback Method
cpg	1034.43	J/mol×K	1187.13	Joback Method
cpg	1039.34	J/mol×K	1226.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392126&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