Glutaric acid, hex-4-yn-3-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C20H26O5/c1-5-10-16(6-2)24-19(21)13-9-14-20(22)25-18-12-8-7-11-17(18)23

InchiKey: HHSHFXAVSHGRAF-UHFFFAOYSA-N

Formula: C20H26O5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 346.42

Physical Properties

Property code	Value	Unit	Source
gf	-154.62	kJ/mol	Joback Method
hf	-591.15	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.895		Crippen Method
mcvol	281.050	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	871.78	K	Joback Method
tc	1088.43	K	Joback Method
tf	596.75	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.49	J/mol×K	871.78	Joback Method
cpg	870.58	J/mol×K	907.89	Joback Method
cpg	884.35	J/mol×K	944.00	Joback Method
cpg	896.78	J/mol×K	980.10	Joback Method
cpg	907.90	J/mol×K	1016.21	Joback Method
cpg	917.72	J/mol×K	1052.32	Joback Method
cpg	926.22	J/mol×K	1088.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391871&Units=SI

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