Glutaric acid, hex-4-yn-3-yl (2-naphthyl)methyl ester

Inchi: InChI=1S/C22H24O4/c1-3-8-20(4-2)26-22(24)12-7-11-21(23)25-16-17-13-14-18-9-5-6-10

InchiKey: TZEMLAQECHQFNH-UHFFFAOYSA-N

Formula: C22H24O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	76.31	kJ/mol	Joback Method
hf	-303.86	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.398		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2829.00		NIST Webbook
rinpol	2829.00		NIST Webbook
tb	914.54	K	Joback Method
tc	1143.12	K	Joback Method
tf	644.76	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.91	J/mol×K	914.54	Joback Method
cpg	880.24	J/mol×K	952.64	Joback Method
cpg	893.40	J/mol×K	990.73	Joback Method
cpg	905.46	J/mol×K	1028.83	Joback Method
cpg	916.47	J/mol×K	1066.93	Joback Method
cpg	926.49	J/mol×K	1105.03	Joback Method
cpg	935.59	J/mol×K	1143.12	Joback Method

Sources

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=U392200&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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