Glutaric acid, di(2-methyloct-5-yn-4-yl) ester

Inchi: InChI=1S/C23H36O4/c1-7-9-12-20(16-18(3)4)26-22(24)14-11-15-23(25)27-21(13-10-8-2
InchiKey: DIFUAHJLIWCQQI-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCCC(=O)OC(C#CCC)CC(C)C
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	70.78	kJ/mol	Joback Method
hf	-484.17	kJ/mol	Joback Method
hfus	53.05	kJ/mol	Joback Method
hvap	87.86	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.899		Crippen Method
mcvol	332.610	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	3477.00		NIST Webbook
rinpol	3477.00		NIST Webbook
tb	894.46	K	Joback Method
tc	1104.25	K	Joback Method
tf	645.49	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.67	J/mol×K	894.46	Joback Method
cpg	1069.30	J/mol×K	929.42	Joback Method
cpg	1085.60	J/mol×K	964.39	Joback Method
cpg	1100.60	J/mol×K	999.35	Joback Method
cpg	1114.32	J/mol×K	1034.32	Joback Method
cpg	1126.78	J/mol×K	1069.28	Joback Method
cpg	1138.00	J/mol×K	1104.25	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=U359615&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