Glutaric acid, 3-methylbut-2-en-1-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C22H36O4/c1-4-5-6-7-8-9-10-11-12-13-18-25-21(23)15-14-16-22(24)26-19-17

InchiKey: ONLPKYXJRHTIOZ-UHFFFAOYSA-N

Formula: C22H36O4

SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-59.01	kJ/mol	Joback Method
hf	-607.28	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	85.07	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.353		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1095.72	kPa	Joback Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	868.38	K	Joback Method
tc	1067.28	K	Joback Method
tf	569.08	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.93	J/mol×K	868.38	Joback Method
cpg	1031.51	J/mol×K	901.53	Joback Method
cpg	1048.00	J/mol×K	934.68	Joback Method
cpg	1063.42	J/mol×K	967.83	Joback Method
cpg	1077.80	J/mol×K	1000.98	Joback Method
cpg	1091.20	J/mol×K	1034.13	Joback Method
cpg	1103.62	J/mol×K	1067.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393942&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