Glutaric acid, 2-methylpent-3-yl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C20H34O4/c1-7-9-11-17(14-15(3)4)23-19(21)12-10-13-20(22)24-18(8-2)16(5)6

InchiKey: HTNQDVJAKXIRAO-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-157.28	kJ/mol	Joback Method
hf	-694.55	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.506		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	816.82	K	Joback Method
tc	1013.78	K	Joback Method
tf	505.58	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.79	J/mol×K	816.82	Joback Method
cpg	939.68	J/mol×K	849.65	Joback Method
cpg	956.42	J/mol×K	882.47	Joback Method
cpg	972.04	J/mol×K	915.30	Joback Method
cpg	986.53	J/mol×K	948.13	Joback Method
cpg	999.94	J/mol×K	980.95	Joback Method
cpg	1012.26	J/mol×K	1013.78	Joback Method

Sources

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=U394018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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