Glutaric acid, isohexyl 2-methyloct-5-yn-4-yl ester

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

InchiKey: TVOQNVJJRLZJCU-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-154.84	kJ/mol	Joback Method
hf	-689.27	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.507		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	3410.00		NIST Webbook
tb	817.26	K	Joback Method
tc	1012.46	K	Joback Method
tf	520.58	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.30	J/mol×K	817.26	Joback Method
cpg	939.03	J/mol×K	849.79	Joback Method
cpg	955.64	J/mol×K	882.33	Joback Method
cpg	971.16	J/mol×K	914.86	Joback Method
cpg	985.59	J/mol×K	947.39	Joback Method
cpg	998.96	J/mol×K	979.93	Joback Method
cpg	1011.27	J/mol×K	1012.46	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=U359602&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