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

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

InchiKey: JWIORUWBFFYUTH-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-152.40	kJ/mol	Joback Method
hf	-683.99	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.652		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	3425.00		NIST Webbook
rinpol	3425.00		NIST Webbook
tb	817.70	K	Joback Method
tc	1011.28	K	Joback Method
tf	535.58	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.80	J/mol×K	817.70	Joback Method
cpg	938.39	J/mol×K	849.96	Joback Method
cpg	954.89	J/mol×K	882.23	Joback Method
cpg	970.32	J/mol×K	914.49	Joback Method
cpg	984.69	J/mol×K	946.75	Joback Method
cpg	998.02	J/mol×K	979.02	Joback Method
cpg	1010.33	J/mol×K	1011.28	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=U359603&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

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