Glutaric acid, hexyl non-5-yn-3-yl ester

Inchi: InChI=1S/C20H34O4/c1-4-7-9-11-14-18(6-3)24-20(22)16-13-15-19(21)23-17-12-10-8-5-2
InchiKey: OMIRELRNVNEEGQ-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCC
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-149.96	kJ/mol	Joback Method
hf	-678.71	kJ/mol	Joback Method
hfus	52.73	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.796		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	818.14	K	Joback Method
tc	1010.24	K	Joback Method
tf	550.58	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.30	J/mol×K	818.14	Joback Method
cpg	937.76	J/mol×K	850.16	Joback Method
cpg	954.15	J/mol×K	882.17	Joback Method
cpg	969.50	J/mol×K	914.19	Joback Method
cpg	983.82	J/mol×K	946.20	Joback Method
cpg	997.13	J/mol×K	978.22	Joback Method
cpg	1009.43	J/mol×K	1010.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359803&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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