Glutaric acid, hex-4-yn-3-yl pentyl ester

Inchi: InChI=1S/C16H26O4/c1-4-7-8-13-19-15(17)11-9-12-16(18)20-14(6-3)10-5-2/h14H,4,6-9,
InchiKey: MEHFEZQBGIOPJU-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-183.64	kJ/mol	Joback Method
hf	-596.15	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.235		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	1960.00		NIST Webbook
tb	726.62	K	Joback Method
tc	918.00	K	Joback Method
tf	505.50	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.55	J/mol×K	726.62	Joback Method
cpg	704.73	J/mol×K	758.52	Joback Method
cpg	720.03	J/mol×K	790.41	Joback Method
cpg	734.46	J/mol×K	822.31	Joback Method
cpg	748.04	J/mol×K	854.21	Joback Method
cpg	760.75	J/mol×K	886.10	Joback Method
cpg	772.61	J/mol×K	918.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359856&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

Latest version available from:
https://www.chemeo.com/cid/42-722-3/Glutaric-acid-hex-4-yn-3-yl-pentyl-ester.pdf
Generated by Cheméo on 2024-10-12 05:45:50.453594415 +0000 UTC m=+3292813.090563662.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.