Glutaric acid, hex-4-yn-3-yl 4-methylpent-2-yl ester

Inchi: InChI=1S/C17H28O4/c1-6-9-15(7-2)21-17(19)11-8-10-16(18)20-14(5)12-13(3)4/h13-15H

InchiKey: ZAOOWGXPFRSOMW-UHFFFAOYSA-N

Formula: C17H28O4

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

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-180.10	kJ/mol	Joback Method
hf	-627.35	kJ/mol	Joback Method
hfus	37.91	kJ/mol	Joback Method
hvap	72.74	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.480		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	748.62	K	Joback Method
tc	944.19	K	Joback Method
tf	486.77	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.01	J/mol×K	748.62	Joback Method
cpg	762.99	J/mol×K	781.21	Joback Method
cpg	778.98	J/mol×K	813.81	Joback Method
cpg	794.00	J/mol×K	846.40	Joback Method
cpg	808.06	J/mol×K	879.00	Joback Method
cpg	821.15	J/mol×K	911.59	Joback Method
cpg	833.29	J/mol×K	944.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392488&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