Glutaric acid, 3-methylbut-2-en-1-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H24O4/c1-5-8-14(6-2)20-16(18)10-7-9-15(17)19-12-11-13(3)4/h11,14H,6-7

InchiKey: JCFQXMXZIZYBOK-UHFFFAOYSA-N

Formula: C16H24O4

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

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-111.97	kJ/mol	Joback Method
hf	-488.72	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.011		Crippen Method
mcvol	238.280	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	730.66	K	Joback Method
tc	930.21	K	Joback Method
tf	486.46	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.55	J/mol×K	730.66	Joback Method
cpg	680.41	J/mol×K	763.92	Joback Method
cpg	695.38	J/mol×K	797.18	Joback Method
cpg	709.47	J/mol×K	830.44	Joback Method
cpg	722.71	J/mol×K	863.69	Joback Method
cpg	735.11	J/mol×K	896.95	Joback Method
cpg	746.68	J/mol×K	930.21	Joback Method

Sources

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=U393975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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