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

Inchi: InChI=1S/C18H26O4/c1-3-6-15(4-2)21-17(19)7-5-8-18(20)22-16-12-13-9-10-14(16)11-13
InchiKey: QIOXUKQQTORIAU-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC1CC2CCC1C2
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-65.11	kJ/mol	Joback Method
hf	-518.33	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.234		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2171.00		NIST Webbook
rinpol	2171.00		NIST Webbook
tb	785.46	K	Joback Method
tc	997.81	K	Joback Method
tf	556.16	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.74	J/mol×K	785.46	Joback Method
cpg	795.80	J/mol×K	820.85	Joback Method
cpg	812.69	J/mol×K	856.24	Joback Method
cpg	828.46	J/mol×K	891.63	Joback Method
cpg	843.16	J/mol×K	927.02	Joback Method
cpg	856.85	J/mol×K	962.41	Joback Method
cpg	869.58	J/mol×K	997.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405490&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