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

Inchi: InChI=1S/C18H32O4/c1-14(2)10-11-21-16(19)8-7-9-17(20)22-13-15(3)12-18(4,5)6/h10,1

InchiKey: PMCWOUNJQXWEOH-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-295.09	kJ/mol	Joback Method
hf	-811.05	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.282		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	764.19	K	Joback Method
tc	954.49	K	Joback Method
tf	405.32	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.94	J/mol×K	764.19	Joback Method
cpg	844.31	J/mol×K	795.91	Joback Method
cpg	860.69	J/mol×K	827.62	Joback Method
cpg	876.13	J/mol×K	859.34	Joback Method
cpg	890.66	J/mol×K	891.06	Joback Method
cpg	904.32	J/mol×K	922.77	Joback Method
cpg	917.14	J/mol×K	954.49	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=U391528&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