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

Inchi: InChI=1S/C17H30O4/c1-12(2)10-11-20-15(18)8-7-9-16(19)21-17(13(3)4)14(5)6/h10,13-1
InchiKey: VUHSGQPPQFIUPZ-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CC(C)=CCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-311.23	kJ/mol	Joback Method
hf	-792.22	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.890		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	743.66	K	Joback Method
tc	932.47	K	Joback Method
tf	361.63	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.43	J/mol×K	743.66	Joback Method
cpg	785.63	J/mol×K	775.13	Joback Method
cpg	801.88	J/mol×K	806.60	Joback Method
cpg	817.21	J/mol×K	838.07	Joback Method
cpg	831.62	J/mol×K	869.54	Joback Method
cpg	845.15	J/mol×K	901.00	Joback Method
cpg	857.82	J/mol×K	932.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393475&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

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