Glutaric acid, 2-(cyclohexyl)ethyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C18H30O4/c1-15(2)11-13-21-17(19)9-6-10-18(20)22-14-12-16-7-4-3-5-8-16/h1

InchiKey: VCZYIPXQPKZSJS-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-271.04	kJ/mol	Joback Method
hf	-742.70	kJ/mol	Joback Method
hfus	38.68	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.180		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	787.41	K	Joback Method
tc	989.30	K	Joback Method
tf	425.28	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.79	J/mol×K	787.41	Joback Method
cpg	839.15	J/mol×K	821.06	Joback Method
cpg	856.29	J/mol×K	854.71	Joback Method
cpg	872.27	J/mol×K	888.36	Joback Method
cpg	887.09	J/mol×K	922.00	Joback Method
cpg	900.80	J/mol×K	955.65	Joback Method
cpg	913.43	J/mol×K	989.30	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=U405417&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

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