

Glutaric acid, di(2,2-dimethylpent-3-yl) ester

Inchi: InChI=1S/C19H36O4/c1-9-14(18(3,4)5)22-16(20)12-11-13-17(21)23-15(10-2)19(6,7)8/h1
InchiKey: JCUJZCJZAPSBDS-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCC(OC(=O)CCCC(=O)OC(CC)C(C)(C)C)C(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-357.94	kJ/mol	Joback Method
hf	-953.15	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.893		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2155.00		NIST Webbook
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tb	779.36	K	Joback Method
tc	971.10	K	Joback Method
tf	423.05	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.49	J/molxK	779.36	Joback Method
cpg	993.96	J/molxK	939.15	Joback Method
cpg	979.69	J/molxK	907.19	Joback Method
cpg	964.46	J/molxK	875.23	Joback Method
cpg	948.21	J/molxK	843.27	Joback Method
cpg	930.90	J/molxK	811.32	Joback Method
cpg	1007.30	J/molxK	971.10	Joback Method
dvisc	0.0000341	Paxs	779.36	Joback Method

dvisc	0.0000489	Paxs	719.98	Joback Method
dvisc	0.0000747	Paxs	660.59	Joback Method
dvisc	0.0001240	Paxs	601.20	Joback Method
dvisc	0.0002302	Paxs	541.82	Joback Method
dvisc	0.0004975	Paxs	482.43	Joback Method
dvisc	0.0013351	Paxs	423.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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