

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

Inchi: InChI=1S/C17H32O4/c1-11(2)14(7)20-15(18)9-8-10-16(19)21-17(12(3)4)13(5)6/h11-14,1
InchiKey: QXMPUFLEUOOPJW-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CC(C)C(C)OC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-387.78	kJ/mol	Joback Method
hf	-910.21	kJ/mol	Joback Method
hfus	27.75	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.968		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	1782.00		NIST Webbook
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tb	738.74	K	Joback Method
tc	925.22	K	Joback Method
tf	350.67	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.45	J/molxK	738.74	Joback Method
cpg	873.40	J/molxK	894.14	Joback Method
cpg	859.36	J/molxK	863.06	Joback Method
cpg	844.36	J/molxK	831.98	Joback Method
cpg	828.38	J/molxK	800.90	Joback Method
cpg	811.41	J/molxK	769.82	Joback Method
cpg	886.48	J/molxK	925.22	Joback Method
dvisc	0.0000542	Paxs	738.74	Joback Method

dvisc	0.0000783	Paxs	674.06	Joback Method
dvisc	0.0001224	Paxs	609.38	Joback Method
dvisc	0.0002127	Paxs	544.70	Joback Method
dvisc	0.0004290	Paxs	480.03	Joback Method
dvisc	0.0010768	Paxs	415.35	Joback Method
dvisc	0.0037951	Paxs	350.67	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=U393473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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