

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

Inchi:	InChI=1S/C16H30O4/c1-11(2)10-19-14(17)8-7-9-15(18)20-16(12(3)4)13(5)6/h11-13,16H
InchiKey:	UXHICLNPNLKXQI-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CC(C)COC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-393.76	kJ/mol	Joback Method
hf	-884.29	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.580		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1802.00		NIST Webbook
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tb	716.30	K	Joback Method
tc	900.82	K	Joback Method
tf	354.40	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.52	J/mol×K	716.30	Joback Method
cpg	752.94	J/mol×K	747.05	Joback Method
cpg	769.44	J/mol×K	777.81	Joback Method
cpg	785.03	J/mol×K	808.56	Joback Method
cpg	799.71	J/mol×K	839.31	Joback Method
cpg	813.48	J/mol×K	870.06	Joback Method
cpg	826.37	J/mol×K	900.82	Joback Method
dvisc	0.0031943	Pa×s	354.40	Joback Method

dvisc	0.0010527	Pa×s	414.72	Joback Method
dvisc	0.0004599	Pa×s	475.03	Joback Method
dvisc	0.0002421	Pa×s	535.35	Joback Method
dvisc	0.0001452	Pa×s	595.67	Joback Method
dvisc	0.0000956	Pa×s	655.98	Joback Method
dvisc	0.0000676	Pa×s	716.30	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=U359474&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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