

Glutaric acid, 2,5-dimethylphenyl propyl ester

Inchi:	InChI=1S/C16H22O4/c1-4-10-19-15(17)6-5-7-16(18)20-14-11-12(2)8-9-13(14)3/h8-9,11H
InchiKey:	QLZBQJCDWLORNN-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCCOC(=O)CCCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-290.85	kJ/mol	Joback Method
hf	-649.58	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.332		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	754.70	K	Joback Method
tc	957.28	K	Joback Method
tf	465.86	K	Joback Method
vc	0.872	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.65	J/molxK	754.70	Joback Method
cpg	662.66	J/molxK	788.46	Joback Method
cpg	676.72	J/molxK	822.23	Joback Method
cpg	689.83	J/molxK	855.99	Joback Method
cpg	702.00	J/molxK	889.75	Joback Method
cpg	713.22	J/molxK	923.52	Joback Method
cpg	723.52	J/molxK	957.28	Joback Method
dvisc	0.0007216	Paxs	465.86	Joback Method

dvisc	0.0004379	Paxs	514.00	Joback Method
dvisc	0.0002895	Paxs	562.14	Joback Method
dvisc	0.0002043	Paxs	610.28	Joback Method
dvisc	0.0001517	Paxs	658.42	Joback Method
dvisc	0.0001173	Paxs	706.56	Joback Method
dvisc	0.0000937	Paxs	754.70	Joback Method

Sources

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=U358935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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