

Glutaric acid, 3,4-dimethylphenyl isohexyl ester

Inchi:	InChI=1S/C19H28O4/c1-14(2)7-6-12-22-18(20)8-5-9-19(21)23-17-11-10-15(3)16(4)13-17
InchiKey:	AWBJWFWBZRATEL-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	<chem>Cc1ccc(OC(=O)CCCC(=O)OCCCC(C)C)cc1C</chem>
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-268.03	kJ/mol	Joback Method
hf	-716.78	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.359		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinsol	2429.00		NIST Webbook
tb	822.90	K	Joback Method
tc	1025.30	K	Joback Method
tf	484.67	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.92	J/molxK	822.90	Joback Method
cpg	834.90	J/molxK	856.63	Joback Method
cpg	849.76	J/molxK	890.37	Joback Method
cpg	863.52	J/molxK	924.10	Joback Method
cpg	876.19	J/molxK	957.83	Joback Method
cpg	887.79	J/molxK	991.56	Joback Method
cpg	898.33	J/molxK	1025.30	Joback Method
dvisc	0.0006296	Paxs	484.67	Joback Method
dvisc	0.0003445	Paxs	541.04	Joback Method

dvisc	0.0002112	Paxs	597.41	Joback Method
dvisc	0.0001409	Paxs	653.78	Joback Method
dvisc	0.0001002	Paxs	710.16	Joback Method
dvisc	0.0000750	Paxs	766.53	Joback Method
dvisc	0.0000584	Paxs	822.90	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=U359181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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