

Glutaric acid, 2,3-dimethylphenyl isobutyl ester

Inchi:	InChI=1S/C17H24O4/c1-12(2)11-20-16(18)9-6-10-17(19)21-15-8-5-7-13(3)14(15)4/h5,7-
InchiKey:	RXVRMZLCIUESRK-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	<chem>Cc1cccc(OC(=O)CCCC(=O)OCC(C)C)c1C</chem>
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-284.87	kJ/mol	Joback Method
hf	-675.50	kJ/mol	Joback Method
hfus	35.10	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.578		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	2177.00		NIST Webbook
tb	777.14	K	Joback Method
tc	981.04	K	Joback Method
tf	462.13	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.13	J/molxK	777.14	Joback Method
cpg	771.51	J/molxK	947.06	Joback Method
cpg	760.06	J/molxK	913.08	Joback Method
cpg	747.62	J/molxK	879.09	Joback Method
cpg	734.15	J/molxK	845.11	Joback Method
cpg	719.66	J/molxK	811.12	Joback Method
cpg	781.95	J/molxK	981.04	Joback Method
dvisc	0.0000760	Paxs	777.14	Joback Method
dvisc	0.0000971	Paxs	724.64	Joback Method

dvisc	0.0001287	Paxs	672.14	Joback Method
dvisc	0.0001789	Paxs	619.63	Joback Method
dvisc	0.0002645	Paxs	567.13	Joback Method
dvisc	0.0004235	Paxs	514.63	Joback Method
dvisc	0.0007546	Paxs	462.13	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=U359297&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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