

Glutaric acid, ethyl 3-methylbenzyl ester

Inchi:	InChI=1S/C15H20O4/c1-3-18-14(16)8-5-9-15(17)19-11-13-7-4-6-12(2)10-13/h4,6-7,10H,
InchiKey:	XRVIJHSEJSSARH-UHFFFAOYSA-N
Formula:	C15H20O4
SMILES:	CCOC(=O)CCCC(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	-289.64	kJ/mol	Joback Method
hf	-617.47	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.772		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	726.84	K	Joback Method
tc	930.46	K	Joback Method
tf	442.07	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.63	J/molxK	726.84	Joback Method
cpg	608.41	J/molxK	760.78	Joback Method
cpg	622.26	J/molxK	794.71	Joback Method
cpg	635.18	J/molxK	828.65	Joback Method
cpg	647.19	J/molxK	862.59	Joback Method
cpg	658.30	J/molxK	896.52	Joback Method
cpg	668.51	J/molxK	930.46	Joback Method
dvisc	0.0009203	Paxs	442.07	Joback Method

dvisc	0.0005387	Paxs	489.53	Joback Method
dvisc	0.0003467	Paxs	536.99	Joback Method
dvisc	0.0002396	Paxs	584.46	Joback Method
dvisc	0.0001751	Paxs	631.92	Joback Method
dvisc	0.0001337	Paxs	679.38	Joback Method
dvisc	0.0001057	Paxs	726.84	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=U377645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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