

Glutaric acid, ethyl 1-phenylethyl ester

Inchi:	InChI=1S/C15H20O4/c1-3-18-14(16)10-7-11-15(17)19-12(2)13-8-5-4-6-9-13/h4-6,8-9,12
InchiKey:	CTQWYVMHBOPPCN-UHFFFAOYSA-N
Formula:	C15H20O4
SMILES:	CCOC(=O)CCCC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	-282.45	kJ/mol	Joback Method
hf	-611.28	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	69.18	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.024		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpola	2037.00		NIST Webbook
tb	721.42	K	Joback Method
tc	927.47	K	Joback Method
tf	414.55	K	Joback Method
vc	0.809	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.99	J/molxK	721.42	Joback Method
cpg	610.15	J/molxK	755.76	Joback Method
cpg	624.31	J/molxK	790.10	Joback Method
cpg	637.50	J/molxK	824.44	Joback Method
cpg	649.73	J/molxK	858.78	Joback Method
cpg	661.01	J/molxK	893.13	Joback Method
cpg	671.36	J/molxK	927.47	Joback Method
dvisc	0.0013106	Paxs	414.55	Joback Method
dvisc	0.0006703	Paxs	465.69	Joback Method

dvisc	0.0003915	Paxs	516.84	Joback Method
dvisc	0.0002519	Paxs	567.99	Joback Method
dvisc	0.0001744	Paxs	619.13	Joback Method
dvisc	0.0001276	Paxs	670.27	Joback Method
dvisc	0.0000977	Paxs	721.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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