

Glutaric acid, ethyl pentyl ester

Inchi:	InChI=1S/C12H22O4/c1-3-5-6-10-16-12(14)9-7-8-11(13)15-4-2/h3-10H2,1-2H3
InchiKey:	BHAKSOAIYLGQLR-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCCCOC(=O)CCCC(=O)OCC
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-417.68	kJ/mol	Joback Method
hf	-780.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.453		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpola	1597.00		NIST Webbook
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tb	626.54	K	Joback Method
tc	803.91	K	Joback Method
tf	369.32	K	Joback Method
vc	0.755	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.96	J/molxK	626.54	Joback Method
cpg	530.51	J/molxK	656.10	Joback Method
cpg	544.42	J/molxK	685.66	Joback Method
cpg	557.71	J/molxK	715.23	Joback Method
cpg	570.37	J/molxK	744.79	Joback Method
cpg	582.39	J/molxK	774.35	Joback Method
cpg	593.78	J/molxK	803.91	Joback Method
dvisc	0.0017118	Paxs	369.32	Joback Method

dvisc	0.0009273	Paxs	412.19	Joback Method
dvisc	0.0005638	Paxs	455.06	Joback Method
dvisc	0.0003735	Paxs	497.93	Joback Method
dvisc	0.0002641	Paxs	540.80	Joback Method
dvisc	0.0001965	Paxs	583.67	Joback Method
dvisc	0.0001522	Paxs	626.54	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=U360002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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