

Glutaric acid, 1-phenylethyl propyl ester

Inchi:	InChI=1S/C16H22O4/c1-3-12-19-15(17)10-7-11-16(18)20-13(2)14-8-5-4-6-9-14/h4-6,8-9
InchiKey:	UFYCTILZYFNLMH-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCCOC(=O)CCCC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-274.03	kJ/mol	Joback Method
hf	-631.92	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	71.41	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.414		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	744.30	K	Joback Method
tc	948.22	K	Joback Method
tf	425.82	K	Joback Method
vc	0.866	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.77	J/molxK	744.30	Joback Method
cpg	665.24	J/molxK	778.29	Joback Method
cpg	679.68	J/molxK	812.27	Joback Method
cpg	693.12	J/molxK	846.26	Joback Method
cpg	705.57	J/molxK	880.25	Joback Method
cpg	717.05	J/molxK	914.23	Joback Method
cpg	727.58	J/molxK	948.22	Joback Method
dvisc	0.0012005	Paxs	425.82	Joback Method
dvisc	0.0006062	Paxs	478.90	Joback Method

dvisc	0.0003509	Paxs	531.98	Joback Method
dvisc	0.0002242	Paxs	585.06	Joback Method
dvisc	0.0001544	Paxs	638.14	Joback Method
dvisc	0.0001126	Paxs	691.22	Joback Method
dvisc	0.0000859	Paxs	744.30	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=U377511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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