

Glutaric acid, isobutyl 1-phenylethyl ester

Inchi:	InChI=1S/C17H24O4/c1-13(2)12-20-16(18)10-7-11-17(19)21-14(3)15-8-5-4-6-9-15/h4-6,
InchiKey:	NDEOYJPFXVAZSK-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CC(C)COC(=O)CCCC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-268.05	kJ/mol	Joback Method
hf	-657.84	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.660		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpola	2208.00		NIST Webbook
tb	766.74	K	Joback Method
tc	971.85	K	Joback Method
tf	422.09	K	Joback Method
vc	0.915	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.16	J/molxK	766.74	Joback Method
cpg	722.12	J/molxK	800.92	Joback Method
cpg	736.98	J/molxK	835.11	Joback Method
cpg	750.76	J/molxK	869.29	Joback Method
cpg	763.50	J/molxK	903.48	Joback Method
cpg	775.20	J/molxK	937.66	Joback Method
cpg	785.90	J/molxK	971.85	Joback Method
dvisc	0.0013048	Paxs	422.09	Joback Method
dvisc	0.0005967	Paxs	479.53	Joback Method

dvisc	0.0003226	Paxs	536.97	Joback Method
dvisc	0.0001964	Paxs	594.41	Joback Method
dvisc	0.0001305	Paxs	651.86	Joback Method
dvisc	0.0000927	Paxs	709.30	Joback Method
dvisc	0.0000693	Paxs	766.74	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=U377512&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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