

Glutaric acid, butyl 1-phenylethyl ester

Inchi:	InChI=1S/C17H24O4/c1-3-4-13-20-16(18)11-8-12-17(19)21-14(2)15-9-6-5-7-10-15/h5-7,
InchiKey:	GVPCWSRHGRQQPY-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCCCOC(=O)CCCC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-265.61	kJ/mol	Joback Method
hf	-652.56	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.804		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinqol	2254.00		NIST Webbook
tb	767.18	K	Joback Method
tc	969.48	K	Joback Method
tf	437.09	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.62	J/molxK	767.18	Joback Method
cpg	721.35	J/molxK	800.90	Joback Method
cpg	736.03	J/molxK	834.61	Joback Method
cpg	749.67	J/molxK	868.33	Joback Method
cpg	762.30	J/molxK	902.04	Joback Method
cpg	773.93	J/molxK	935.76	Joback Method
cpg	784.60	J/molxK	969.48	Joback Method
dvisc	0.0010935	Paxs	437.09	Joback Method
dvisc	0.0005455	Paxs	492.11	Joback Method

dvisc	0.0003130	Paxs	547.12	Joback Method
dvisc	0.0001988	Paxs	602.13	Joback Method
dvisc	0.0001362	Paxs	657.15	Joback Method
dvisc	0.0000989	Paxs	712.16	Joback Method
dvisc	0.0000752	Paxs	767.18	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=U377513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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