

Glutaric acid, butyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C17H24O5/c1-2-3-12-21-16(18)10-7-11-17(19)22-14-13-20-15-8-5-4-6-9-15/h
InchiKey:	IOXLLSNLENBQLB-UHFFFAOYSA-N
Formula:	C17H24O5
SMILES:	CCCCOC(=O)CCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	308.37

Physical Properties

Property code	Value	Unit	Source
gf	-368.17	kJ/mol	Joback Method
hf	-779.50	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.122		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpola	2297.00		NIST Webbook
tb	790.04	K	Joback Method
tc	989.47	K	Joback Method
tf	474.32	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.48	J/molxK	790.04	Joback Method
cpg	748.59	J/molxK	823.28	Joback Method
cpg	762.65	J/molxK	856.52	Joback Method
cpg	775.65	J/molxK	889.76	Joback Method
cpg	787.62	J/molxK	922.99	Joback Method
cpg	798.55	J/molxK	956.23	Joback Method
cpg	808.46	J/molxK	989.47	Joback Method
dvisc	0.0006571	Paxs	474.32	Joback Method
dvisc	0.0003642	Paxs	526.94	Joback Method

dvisc	0.0002247	Paxs	579.56	Joback Method
dvisc	0.0001502	Paxs	632.18	Joback Method
dvisc	0.0001068	Paxs	684.80	Joback Method
dvisc	0.0000798	Paxs	737.42	Joback Method
dvisc	0.0000619	Paxs	790.04	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=U376915&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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