

Glutaric acid, butyl 3-methylbenzyl ester

Inchi:	InChI=1S/C17H24O4/c1-3-4-11-20-16(18)9-6-10-17(19)21-13-15-8-5-7-14(2)12-15/h5,7-
InchiKey:	KHKRLGRTYIDNHZ-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCCCOC(=O)CCCC(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.80	kJ/mol	Joback Method
hf	-658.75	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.552		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2391.00		NIST Webbook
tb	772.60	K	Joback Method
tc	973.04	K	Joback Method
tf	464.61	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.35	J/molxK	772.60	Joback Method
cpg	771.51	J/molxK	939.63	Joback Method
cpg	760.03	J/molxK	906.23	Joback Method
cpg	747.59	J/molxK	872.82	Joback Method
cpg	734.18	J/molxK	839.41	Joback Method
cpg	719.77	J/molxK	806.01	Joback Method
cpg	782.03	J/molxK	973.04	Joback Method
dvisc	0.0000821	Paxs	772.60	Joback Method
dvisc	0.0001047	Paxs	721.27	Joback Method

dvisc	0.0001384	Paxs	669.94	Joback Method
dvisc	0.0001917	Paxs	618.61	Joback Method
dvisc	0.0002816	Paxs	567.27	Joback Method
dvisc	0.0004467	Paxs	515.94	Joback Method
dvisc	0.0007844	Paxs	464.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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