

Glutaric acid, butyl 1-phenylpropyl ester

Inchi:	InChI=1S/C18H26O4/c1-3-5-14-21-17(19)12-9-13-18(20)22-16(4-2)15-10-7-6-8-11-15/h6
InchiKey:	FUCZVGTVOBBDTP-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-257.19	kJ/mol	Joback Method
hf	-673.20	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.194		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpola	2170.00		NIST Webbook
tb	790.06	K	Joback Method
tc	991.28	K	Joback Method
tf	448.36	K	Joback Method
vc	0.978	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.47	J/molxK	790.06	Joback Method
cpg	831.62	J/molxK	957.74	Joback Method
cpg	819.87	J/molxK	924.21	Joback Method
cpg	807.11	J/molxK	890.67	Joback Method
cpg	793.30	J/molxK	857.13	Joback Method
cpg	778.43	J/molxK	823.60	Joback Method
cpg	842.38	J/molxK	991.28	Joback Method
dvisc	0.0000657	Paxs	790.06	Joback Method
dvisc	0.0000866	Paxs	733.11	Joback Method

dvisc	0.0001197	Paxs	676.16	Joback Method
dvisc	0.0001755	Paxs	619.21	Joback Method
dvisc	0.0002780	Paxs	562.26	Joback Method
dvisc	0.0004886	Paxs	505.31	Joback Method
dvisc	0.0009909	Paxs	448.36	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=U358950&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
mccvol:	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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