

Diglycolic acid, butyl 2-methylphenyl ester

Inchi:	InChI=1S/C15H20O5/c1-3-4-9-19-14(16)10-18-11-15(17)20-13-8-6-5-7-12(13)2/h5-8H,3
InchiKey:	QGWJLQPCQFAG-UHFFFAOYSA-N
Formula:	C15H20O5
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccccc1C
Mol. weight [g/mol]:	280.32

Physical Properties

Property code	Value	Unit	Source
gf	-394.64	kJ/mol	Joback Method
hf	-749.69	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.260		Crippen Method
mvol	219.200	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	749.26	K	Joback Method
tc	951.78	K	Joback Method
tf	464.30	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.91	J/molxK	749.26	Joback Method
cpg	635.35	J/molxK	783.01	Joback Method
cpg	648.83	J/molxK	816.77	Joback Method
cpg	661.35	J/molxK	850.52	Joback Method
cpg	672.91	J/molxK	884.27	Joback Method
cpg	683.50	J/molxK	918.02	Joback Method
cpg	693.12	J/molxK	951.78	Joback Method
dvisc	0.0006625	Paxs	464.30	Joback Method

dvisc	0.0003969	Paxs	511.79	Joback Method
dvisc	0.0002594	Paxs	559.29	Joback Method
dvisc	0.0001812	Paxs	606.78	Joback Method
dvisc	0.0001333	Paxs	654.27	Joback Method
dvisc	0.0001023	Paxs	701.77	Joback Method
dvisc	0.0000811	Paxs	749.26	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=U382006&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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