

Diglycolic acid, 4-acetylphenyl butyl ester

Inchi:	InChI=1S/C16H20O6/c1-3-4-9-21-15(18)10-20-11-16(19)22-14-7-5-13(6-8-14)12(2)17/h5
InchiKey:	CTUVRDMUYYLUIL-UHFFFAOYSA-N
Formula:	C16H20O6
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	308.33

Physical Properties

Property code	Value	Unit	Source
gf	-515.14	kJ/mol	Joback Method
hf	-882.91	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.154		Crippen Method
mvol	234.860	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	826.01	K	Joback Method
tc	1034.00	K	Joback Method
tf	525.50	K	Joback Method
vc	0.895	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.41	J/molxK	826.01	Joback Method
cpg	704.43	J/molxK	860.67	Joback Method
cpg	716.36	J/molxK	895.34	Joback Method
cpg	727.21	J/molxK	930.00	Joback Method
cpg	736.96	J/molxK	964.67	Joback Method
cpg	745.62	J/molxK	999.33	Joback Method
cpg	753.18	J/molxK	1034.00	Joback Method
dvisc	0.0005159	Paxs	525.50	Joback Method

dvisc	0.0003189	Paxs	575.59	Joback Method
dvisc	0.0002130	Paxs	625.67	Joback Method
dvisc	0.0001510	Paxs	675.75	Joback Method
dvisc	0.0001122	Paxs	725.84	Joback Method
dvisc	0.0000867	Paxs	775.92	Joback Method
dvisc	0.0000691	Paxs	826.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	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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