

Diglycolic acid, 2-acetylphenyl nonyl ester

Inchi:

InChI=1S/C21H30O6/c1-3-4-5-6-7-8-11-14-26-20(23)15-25-16-21(24)27-19-13-10-9-12-1

InchiKey:

AUASJECXPJNKEA-UHFFFAOYSA-N

Formula:

C21H30O6

SMILES:

CCCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O

Mol. weight [g/mol]:

378.46

Physical Properties

Property code	Value	Unit	Source
gf	-473.04	kJ/mol	Joback Method
hf	-986.11	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	92.75	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.105		Crippen Method
mcvol	305.310	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	3331.00		NIST Webbook
tb	940.41	K	Joback Method
tc	1153.53	K	Joback Method
tf	581.85	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.33	J/mol×K	940.41	Joback Method
cpg	995.16	J/mol×K	975.93	Joback Method
cpg	1007.58	J/mol×K	1011.45	Joback Method
cpg	1018.62	J/mol×K	1046.97	Joback Method
cpg	1028.29	J/mol×K	1082.49	Joback Method
cpg	1036.61	J/mol×K	1118.01	Joback Method
cpg	1043.57	J/mol×K	1153.53	Joback Method
dvisc	0.0003079	Pa×s	581.85	Joback Method
dvisc	0.0001794	Pa×s	641.61	Joback Method

dvisc	0.0001146	Pa×s	701.37	Joback Method
dvisc	0.0000785	Pa×s	761.13	Joback Method
dvisc	0.0000569	Pa×s	820.89	Joback Method
dvisc	0.0000430	Pa×s	880.65	Joback Method
dvisc	0.0000337	Pa×s	940.41	Joback Method

Sources

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=U382725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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