Diglycolic acid, butyl 2-formylphenyl ester

Inchi: InChI=1S/C15H18O6/c1-2-3-8-20-14(17)10-19-11-15(18)21-13-7-5-4-6-12(13)9-16/h4-7,
InchiKey: XGALRCKVSXWZNI-UHFFFAOYSA-N
Formula: C15H18O6
SMILES: CCCCOC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
gf	-494.16	kJ/mol	Joback Method
hf	-835.27	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.764		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	797.92	K	Joback Method
tc	1003.87	K	Joback Method
tf	506.30	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.85	J/mol×K	797.92	Joback Method
cpg	648.49	J/mol×K	832.25	Joback Method
cpg	660.15	J/mol×K	866.57	Joback Method
cpg	670.80	J/mol×K	900.90	Joback Method
cpg	680.46	J/mol×K	935.22	Joback Method
cpg	689.11	J/mol×K	969.55	Joback Method
cpg	696.76	J/mol×K	1003.87	Joback Method
dvisc	0.0006475	Pa×s	506.30	Joback Method

dvisc	0.0004019	Pa×s	554.90	Joback Method
dvisc	0.0002694	Pa×s	603.51	Joback Method
dvisc	0.0001917	Pa×s	652.11	Joback Method
dvisc	0.0001430	Pa×s	700.71	Joback Method
dvisc	0.0001108	Pa×s	749.32	Joback Method
dvisc	0.0000885	Pa×s	797.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U382309&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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