

Diglycolic acid, 2-formylphenyl heptyl ester

Inchi:	InChI=1S/C18H24O6/c1-2-3-4-5-8-11-23-17(20)13-22-14-18(21)24-16-10-7-6-9-15(16)12
InchiKey:	SNWUQMFOXSICCY-UHFFFAOYSA-N
Formula:	C18H24O6
SMILES:	CCCCCCCOC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]:	336.38

Physical Properties

Property code	Value	Unit	Source
gf	-468.90	kJ/mol	Joback Method
hf	-897.19	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	86.04	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.935		Crippen Method
mvol	263.040	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	3096.00		NIST Webbook
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tb	866.56	K	Joback Method
tc	1071.90	K	Joback Method
tf	540.11	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.06	J/molxK	866.56	Joback Method
cpg	818.44	J/molxK	900.78	Joback Method
cpg	830.66	J/molxK	935.01	Joback Method
cpg	841.73	J/molxK	969.23	Joback Method
cpg	851.67	J/molxK	1003.45	Joback Method
cpg	860.47	J/molxK	1037.68	Joback Method
cpg	868.14	J/molxK	1071.90	Joback Method
dvisc	0.0004888	Paxs	540.11	Joback Method

dvisc	0.0002921	Paxs	594.52	Joback Method
dvisc	0.0001903	Paxs	648.93	Joback Method
dvisc	0.0001325	Paxs	703.34	Joback Method
dvisc	0.0000971	Paxs	757.74	Joback Method
dvisc	0.0000742	Paxs	812.15	Joback Method
dvisc	0.0000587	Paxs	866.56	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=U382313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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