

Diglycolic acid, 2-chlorophenyl heptyl ester

Inchi: InChI=1S/C17H23ClO5/c1-2-3-4-5-8-11-22-16(19)12-21-13-17(20)23-15-10-7-6-9-14(15)
InchiKey: JSOCGVFNZDQOMM-UHFFFAOYSA-N
Formula: C17H23ClO5
SMILES: CCCCCCOC(=O)COCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-389.73	kJ/mol	Joback Method
hf	-806.71	kJ/mol	Joback Method
hfus	44.40	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.776		Crippen Method
mvol	259.620	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rmpol	2974.00		NIST Webbook
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tb	832.45	K	Joback Method
tc	1037.10	K	Joback Method
tf	516.76	K	Joback Method
vc	0.995	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.04	J/molxK	832.45	Joback Method
cpg	772.88	J/molxK	866.56	Joback Method
cpg	785.64	J/molxK	900.67	Joback Method
cpg	797.31	J/molxK	934.78	Joback Method
cpg	807.90	J/molxK	968.88	Joback Method
cpg	817.41	J/molxK	1002.99	Joback Method
cpg	825.85	J/molxK	1037.10	Joback Method
dvisc	0.0004644	Paxs	516.76	Joback Method

dvisc	0.0002753	Paxs	569.38	Joback Method
dvisc	0.0001783	Paxs	621.99	Joback Method
dvisc	0.0001236	Paxs	674.61	Joback Method
dvisc	0.0000903	Paxs	727.22	Joback Method
dvisc	0.0000689	Paxs	779.83	Joback Method
dvisc	0.0000543	Paxs	832.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381975&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
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

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