Diglycolic acid, heptyl 4-methoxyphenyl ester

Inchi: InChI=1S/C18H26O6/c1-3-4-5-6-7-12-23-17(19)13-22-14-18(20)24-16-10-8-15(21-2)9-11
InchiKey: UFRLMYRZDRMTIG-UHFFFAOYSA-N
Formula: C18H26O6
SMILES: CCCCCCCOC(=O)COCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-474.38	kJ/mol	Joback Method
hf	-943.83	kJ/mol	Joback Method
hfus	43.98	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.131		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	840.32	K	Joback Method
tc	1041.15	K	Joback Method
tf	520.34	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.63	J/mol×K	840.32	Joback Method
cpg	833.41	J/mol×K	873.79	Joback Method
cpg	847.00	J/mol×K	907.26	Joback Method
cpg	859.41	J/mol×K	940.74	Joback Method
cpg	870.62	J/mol×K	974.21	Joback Method
cpg	880.63	J/mol×K	1007.68	Joback Method
cpg	889.43	J/mol×K	1041.15	Joback Method
dvisc	0.0003593	Pa×s	520.34	Joback Method

dvisc	0.0002114	Pa×s	573.67	Joback Method
dvisc	0.0001361	Pa×s	627.00	Joback Method
dvisc	0.0000939	Pa×s	680.33	Joback Method
dvisc	0.0000684	Pa×s	733.66	Joback Method
dvisc	0.0000520	Pa×s	786.99	Joback Method
dvisc	0.0000409	Pa×s	840.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381888&Units=SI

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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