Diglycolic acid, 2,5-dimethylphenyl heptyl ester

Inchi: InChI=1S/C19H28O5/c1-4-5-6-7-8-11-23-18(20)13-22-14-19(21)24-17-12-15(2)9-10-16(1

InchiKey: XVOJIYDOALSDJI-UHFFFAOYSA-N

Formula: C19H28O5

SMILES: CCCCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-370.59	kJ/mol	Joback Method
hf	-843.72	kJ/mol	Joback Method
hfus	44.99	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.739		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2957.00		NIST Webbook
tb	845.76	K	Joback Method
tc	1047.04	K	Joback Method
tf	521.90	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.43	J/mol×K	845.76	Joback Method
cpg	912.67	J/mol×K	1013.49	Joback Method
cpg	901.93	J/mol×K	979.95	Joback Method
cpg	890.04	J/mol×K	946.40	Joback Method
cpg	877.00	J/mol×K	912.85	Joback Method
cpg	862.79	J/mol×K	879.31	Joback Method
cpg	922.25	J/mol×K	1047.04	Joback Method
dvisc	0.0000480	Pa×s	845.76	Joback Method
dvisc	0.0000606	Pa×s	791.78	Joback Method

dvisc	0.0000791	Pa×s	737.81	Joback Method
dvisc	0.0001077	Pa×s	683.83	Joback Method
dvisc	0.0001547	Pa×s	629.85	Joback Method
dvisc	0.0002379	Pa×s	575.88	Joback Method
dvisc	0.0003996	Pa×s	521.90	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=U382709&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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