

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(
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
rinqol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.43	J/molxK	845.76	Joback Method
cpg	862.79	J/molxK	879.31	Joback Method
cpg	877.00	J/molxK	912.85	Joback Method
cpg	890.04	J/molxK	946.40	Joback Method
cpg	901.93	J/molxK	979.95	Joback Method
cpg	912.67	J/molxK	1013.49	Joback Method
cpg	922.25	J/molxK	1047.04	Joback Method
dvisc	0.0003996	Paxs	521.90	Joback Method
dvisc	0.0002379	Paxs	575.88	Joback Method

dvisc	0.0001547	Paxs	629.85	Joback Method
dvisc	0.0001077	Paxs	683.83	Joback Method
dvisc	0.0000791	Paxs	737.81	Joback Method
dvisc	0.0000606	Paxs	791.78	Joback Method
dvisc	0.0000480	Paxs	845.76	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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