

Diglycolic acid, heptyl 4-methoxybenzyl ester

Inchi:	InChI=1S/C19H28O6/c1-3-4-5-6-7-12-24-18(20)14-23-15-19(21)25-13-16-8-10-17(22-2)
InchiKey:	HAXMPWJHMKLSIL-UHFFFAOYSA-N
Formula:	C19H28O6
SMILES:	CCCCCCCOC(=O)COCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]:	352.42

Physical Properties

Property code	Value	Unit	Source
gf	-465.96	kJ/mol	Joback Method
hf	-964.47	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.269		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinsol	3309.00		NIST Webbook
tb	863.20	K	Joback Method
tc	1065.06	K	Joback Method
tf	531.61	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.07	J/molxK	863.20	Joback Method
cpg	892.02	J/molxK	896.84	Joback Method
cpg	905.71	J/molxK	930.49	Joback Method
cpg	918.15	J/molxK	964.13	Joback Method
cpg	929.33	J/molxK	997.77	Joback Method
cpg	939.25	J/molxK	1031.42	Joback Method
cpg	947.91	J/molxK	1065.06	Joback Method
dvisc	0.0003244	Paxs	531.61	Joback Method
dvisc	0.0001886	Paxs	586.87	Joback Method

dvisc	0.0001203	Paxs	642.14	Joback Method
dvisc	0.0000825	Paxs	697.40	Joback Method
dvisc	0.0000597	Paxs	752.67	Joback Method
dvisc	0.0000452	Paxs	807.93	Joback Method
dvisc	0.0000355	Paxs	863.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382252&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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