Pimelic acid, hexyl 4-methoxybenzyl ester

Inchi: InChI=1S/C21H32O5/c1-3-4-5-9-16-25-20(22)10-7-6-8-11-21(23)26-17-18-12-14-19(24-2
InchiKey: YPVRQGGFZIHWBK-UHFFFAOYSA-N
Formula: C21H32O5
SMILES: CCCCCCOC(=O)CCCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-344.12	kJ/mol	Joback Method
hf	-873.53	kJ/mol	Joback Method
hfus	50.56	kJ/mol	Joback Method
hvap	86.00	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.812		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1089.96	K	Joback Method
tf	531.92	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/mol×K	886.54	Joback Method
cpg	982.57	J/mol×K	920.44	Joback Method
cpg	997.11	J/mol×K	954.35	Joback Method
cpg	1010.40	J/mol×K	988.25	Joback Method
cpg	1022.43	J/mol×K	1022.15	Joback Method
cpg	1033.23	J/mol×K	1056.05	Joback Method
cpg	1042.80	J/mol×K	1089.96	Joback Method
dvisc	0.0003742	Pa×s	531.92	Joback Method

dvisc	0.0002078	Pa×s	591.02	Joback Method
dvisc	0.0001284	Pa×s	650.13	Joback Method
dvisc	0.0000860	Pa×s	709.23	Joback Method
dvisc	0.0000612	Pa×s	768.33	Joback Method
dvisc	0.0000458	Pa×s	827.44	Joback Method
dvisc	0.0000356	Pa×s	886.54	Joback Method

Sources

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=U416541&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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