Pimelic acid, ethyl 4-methoxybenzyl ester

Inchi: InChI=1S/C17H24O5/c1-3-21-16(18)7-5-4-6-8-17(19)22-13-14-9-11-15(20-2)12-10-14/h9
InchiKey: NADZWKCGXANTNS-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCOC(=O)CCCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-377.80	kJ/mol	Joback Method
hf	-790.97	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.252		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	795.02	K	Joback Method
tc	995.27	K	Joback Method
tf	486.84	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.69	J/mol×K	795.02	Joback Method
cpg	797.27	J/mol×K	961.90	Joback Method
cpg	786.44	J/mol×K	928.52	Joback Method
cpg	774.58	J/mol×K	895.15	Joback Method
cpg	761.66	J/mol×K	861.77	Joback Method
cpg	747.70	J/mol×K	828.40	Joback Method
cpg	807.05	J/mol×K	995.27	Joback Method
dvisc	0.0000624	Pa×s	795.02	Joback Method

dvisc	0.0000792	Pa×s	743.66	Joback Method
dvisc	0.0001043	Pa×s	692.29	Joback Method
dvisc	0.0001434	Pa×s	640.93	Joback Method
dvisc	0.0002084	Pa×s	589.57	Joback Method
dvisc	0.0003254	Pa×s	538.20	Joback Method
dvisc	0.0005581	Pa×s	486.84	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=U416535&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