Pimelic acid, nonyl 3-phenylpropyl ester

Inchi: InChI=1S/C25H40O4/c1-2-3-4-5-6-7-14-21-28-24(26)19-12-9-13-20-25(27)29-22-15-18-2
InchiKey: YHCUEEQFFLMVOH-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-195.81	kJ/mol	Joback Method
hf	-812.40	kJ/mol	Joback Method
hfus	60.12	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.407		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3086.00		NIST Webbook
rinpol	3086.00		NIST Webbook
tb	950.66	K	Joback Method
tc	1163.88	K	Joback Method
tf	542.25	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.85	J/mol×K	950.66	Joback Method
cpg	1255.10	J/mol×K	1128.34	Joback Method
cpg	1243.10	J/mol×K	1092.80	Joback Method
cpg	1229.82	J/mol×K	1057.27	Joback Method
cpg	1215.22	J/mol×K	1021.73	Joback Method
cpg	1199.24	J/mol×K	986.20	Joback Method
cpg	1265.88	J/mol×K	1163.88	Joback Method
dvisc	0.0000259	Pa×s	950.66	Joback Method

dvisc	0.0000343	Pa×s	882.59	Joback Method
dvisc	0.0000475	Pa×s	814.52	Joback Method
dvisc	0.0000697	Pa×s	746.45	Joback Method
dvisc	0.0001106	Pa×s	678.39	Joback Method
dvisc	0.0001945	Pa×s	610.32	Joback Method
dvisc	0.0003943	Pa×s	542.25	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=U416516&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