

Pimelic acid, ethyl 3-phenylpropyl ester

Inchi:	InChI=1S/C18H26O4/c1-2-21-17(19)13-7-4-8-14-18(20)22-15-9-12-16-10-5-3-6-11-16/h3
InchiKey:	UIONKALDTDWGHV-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-254.75	kJ/mol	Joback Method
hf	-667.92	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.676		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	790.50	K	Joback Method
tc	989.35	K	Joback Method
tf	463.36	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.94	J/molxK	790.50	Joback Method
cpg	777.71	J/molxK	823.64	Joback Method
cpg	792.42	J/molxK	856.78	Joback Method
cpg	806.11	J/molxK	889.92	Joback Method
cpg	818.79	J/molxK	923.07	Joback Method
cpg	830.49	J/molxK	956.21	Joback Method
cpg	841.23	J/molxK	989.35	Joback Method
dvisc	0.0008523	Paxs	463.36	Joback Method

dvisc	0.0004537	Paxs	517.88	Joback Method
dvisc	0.0002723	Paxs	572.41	Joback Method
dvisc	0.0001786	Paxs	626.93	Joback Method
dvisc	0.0001253	Paxs	681.45	Joback Method
dvisc	0.0000927	Paxs	735.98	Joback Method
dvisc	0.0000715	Paxs	790.50	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=U416507&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

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