

Pimelic acid, heptyl hexyl ester

Inchi:	InChI=1S/C20H38O4/c1-3-5-7-9-14-18-24-20(22)16-12-10-11-15-19(21)23-17-13-8-6-4-2
InchiKey:	NFSLVMGPCCJTNV-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-350.32	kJ/mol	Joback Method
hf	-945.73	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.574		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
rinpol	1757.00		NIST Webbook
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tb	809.58	K	Joback Method
tc	993.33	K	Joback Method
tf	459.48	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.18	J/molxK	809.58	Joback Method
cpg	987.44	J/molxK	840.20	Joback Method
cpg	1004.65	J/molxK	870.83	Joback Method
cpg	1020.84	J/molxK	901.45	Joback Method
cpg	1036.02	J/molxK	932.08	Joback Method
cpg	1050.21	J/molxK	962.70	Joback Method
cpg	1063.43	J/molxK	993.33	Joback Method
dvisc	0.0008397	Paxs	459.48	Joback Method

dvisc	0.0004093	Paxs	517.83	Joback Method
dvisc	0.0002308	Paxs	576.18	Joback Method
dvisc	0.0001446	Paxs	634.53	Joback Method
dvisc	0.0000980	Paxs	692.88	Joback Method
dvisc	0.0000706	Paxs	751.23	Joback Method
dvisc	0.0000533	Paxs	809.58	Joback Method

Sources

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=U406513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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