

Pimelic acid, 2-methylbutyl octyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-352.76	kJ/mol	Joback Method
hf	-951.01	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	809.14	K	Joback Method
tc	993.61	K	Joback Method
tf	444.48	K	Joback Method
vc	1.198	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.66	J/molxK	809.14	Joback Method
cpg	987.99	J/molxK	839.88	Joback Method
cpg	1005.26	J/molxK	870.63	Joback Method
cpg	1021.49	J/molxK	901.37	Joback Method
cpg	1036.69	J/molxK	932.12	Joback Method
cpg	1050.89	J/molxK	962.86	Joback Method
cpg	1064.10	J/molxK	993.61	Joback Method
dvisc	0.0009916	Paxs	444.48	Joback Method

dvisc	0.0004441	Paxs	505.26	Joback Method
dvisc	0.0002364	Paxs	566.03	Joback Method
dvisc	0.0001422	Paxs	626.81	Joback Method
dvisc	0.0000935	Paxs	687.59	Joback Method
dvisc	0.0000659	Paxs	748.36	Joback Method
dvisc	0.0000489	Paxs	809.14	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=U406651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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