

Pimelic acid, di(methoxydec-4-yl) ester

Inchi:	InChI=1S/C29H56O6/c1-5-7-9-12-18-26(20-16-24-32-3)34-28(30)22-14-11-15-23-29(31)
InchiKey:	FXYOJTZTLLXIKE-UHFFFAOYSA-N
Formula:	C29H56O6
SMILES:	CCCCCCC(CCCOC)OC(=O)CCCCC(=O)OC(CCCCC)CCCOC
Mol. weight [g/mol]:	500.75

Physical Properties

Property code	Value	Unit	Source
gf	-489.42	kJ/mol	Joback Method
hf	-1406.49	kJ/mol	Joback Method
hfus	71.77	kJ/mol	Joback Method
hvap	102.50	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.554		Crippen Method
mvol	446.090	ml/mol	McGowan Method
pc	648.12	kPa	Joback Method
rinpol	3127.00		NIST Webbook
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tb	1059.46	K	Joback Method
tc	1332.23	K	Joback Method
tf	575.37	K	Joback Method
vc	1.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1600.95	J/molxK	1059.46	Joback Method
cpg	1622.00	J/molxK	1104.92	Joback Method
cpg	1639.89	J/molxK	1150.38	Joback Method
cpg	1654.70	J/molxK	1195.84	Joback Method
cpg	1666.46	J/molxK	1241.30	Joback Method
cpg	1675.23	J/molxK	1286.76	Joback Method
cpg	1681.07	J/molxK	1332.23	Joback Method
dvisc	0.0001523	Paxs	575.37	Joback Method

dvisc	0.0000635	Paxs	656.05	Joback Method
dvisc	0.0000320	Paxs	736.73	Joback Method
dvisc	0.0000185	Paxs	817.41	Joback Method
dvisc	0.0000118	Paxs	898.10	Joback Method
dvisc	0.0000081	Paxs	978.78	Joback Method
dvisc	0.0000059	Paxs	1059.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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