

Pimelic acid, isobutyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H26O5/c1-14(2)13-22-17(19)11-5-4-6-12-18(20)23-16-10-8-7-9-15(16)21-3
InchiKey: UJDDCPAGLUFYRO-UHFFFAOYSA-N
Formula: C18H26O5
SMILES: COc1ccccc1OC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-371.82	kJ/mol	Joback Method
hf	-816.89	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.750		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2361.00		NIST Webbook
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tb	817.46	K	Joback Method
tc	1019.56	K	Joback Method
tf	483.11	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.54	J/molxK	817.46	Joback Method
cpg	856.24	J/molxK	985.88	Joback Method
cpg	845.35	J/molxK	952.19	Joback Method
cpg	833.34	J/molxK	918.51	Joback Method
cpg	820.20	J/molxK	884.83	Joback Method
cpg	805.94	J/molxK	851.14	Joback Method
cpg	866.02	J/molxK	1019.56	Joback Method
dvisc	0.0000500	Paxs	817.46	Joback Method

dvisc	0.0000647	Paxs	761.73	Joback Method
dvisc	0.0000872	Paxs	706.01	Joback Method
dvisc	0.0001237	Paxs	650.28	Joback Method
dvisc	0.0001875	Paxs	594.56	Joback Method
dvisc	0.0003097	Paxs	538.84	Joback Method
dvisc	0.0005741	Paxs	483.11	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=U416522&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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