

Pimelic acid, 4-bromo-2-methoxybenzyl propyl ester

Inchi:	InChI=1S/C18H25BrO5/c1-3-11-23-17(20)7-5-4-6-8-18(21)24-13-14-9-10-15(19)12-16(1)
InchiKey:	FTVXVMBVIWHXSI-UHFFFAOYSA-N
Formula:	C18H25BrO5
SMILES:	CCCOC(=O)CCCCC(=O)OCc1ccc(Br)cc1OC
Mol. weight [g/mol]:	401.29

Physical Properties

Property code	Value	Unit	Source
gf	-364.69	kJ/mol	Joback Method
hf	-796.75	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.405		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2649.00		NIST Webbook
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tb	889.04	K	Joback Method
tc	1100.83	K	Joback Method
tf	570.43	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.78	J/molxK	889.04	Joback Method
cpg	841.18	J/molxK	924.34	Joback Method
cpg	853.41	J/molxK	959.64	Joback Method
cpg	864.47	J/molxK	994.93	Joback Method
cpg	874.39	J/molxK	1030.23	Joback Method
cpg	883.16	J/molxK	1065.53	Joback Method
cpg	890.78	J/molxK	1100.83	Joback Method
dvisc	0.0003022	Paxs	570.43	Joback Method

dvisc	0.0001908	Paxs	623.53	Joback Method
dvisc	0.0001295	Paxs	676.63	Joback Method
dvisc	0.0000930	Paxs	729.74	Joback Method
dvisc	0.0000698	Paxs	782.84	Joback Method
dvisc	0.0000544	Paxs	835.94	Joback Method
dvisc	0.0000437	Paxs	889.04	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=U406582&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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