Pimelic acid, 4-bromo-2-methoxybenzyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C21H31BrO5/c1-15(2)12-16(3)27-21(24)9-7-5-6-8-20(23)26-14-17-10-11-18(22

InchiKey: HWDDOFISTYBOGB-UHFFFAOYSA-N

Formula: C21H31BrO5

SMILES: COc1cc(Br)ccc1COC(=O)CCCCCC(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 443.37

Physical Properties

Property code	Value	Unit	Source
gf	-344.31	kJ/mol	Joback Method
hf	-869.23	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.429		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	956.80	K	Joback Method
tc	1175.56	K	Joback Method
tf	574.24	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.52	J/mol×K	956.80	Joback Method
cpg	1019.41	J/mol×K	993.26	Joback Method
cpg	1031.88	J/mol×K	1029.72	Joback Method
cpg	1042.96	J/mol×K	1066.18	Joback Method
cpg	1052.68	J/mol×K	1102.64	Joback Method
cpg	1061.04	J/mol×K	1139.10	Joback Method
cpg	1068.08	J/mol×K	1175.56	Joback Method
dvisc	0.0002530	Pa×s	574.24	Joback Method

dvisc	0.0001391	Pa×s	638.00	Joback Method
dvisc	0.0000853	Pa×s	701.76	Joback Method
dvisc	0.0000567	Pa×s	765.52	Joback Method
dvisc	0.0000401	Pa×s	829.28	Joback Method
dvisc	0.0000299	Pa×s	893.04	Joback Method
dvisc	0.0000231	Pa×s	956.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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