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

Inchi: InChI=1S/C21H31BrO5/c1-3-4-5-9-14-26-20(23)10-7-6-8-11-21(24)27-16-17-12-13-18(22

InchiKey: OMCVAOBOQBTMDP-UHFFFAOYSA-N

Formula: C21H31BrO5

SMILES: CCCCCCOC(=O)CCCCCC(=O)OCc1ccc(Br)cc1OC

Mol. weight [g/mol]: 443.37

Physical Properties

Property code	Value	Unit	Source
gf	-339.43	kJ/mol	Joback Method
hf	-858.67	kJ/mol	Joback Method
hfus	55.46	kJ/mol	Joback Method
hvap	93.10	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.575		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2953.00		NIST Webbook
rinpol	2953.00		NIST Webbook
tb	957.68	K	Joback Method
tc	1174.68	K	Joback Method
tf	604.24	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.65	J/mol×K	957.68	Joback Method
cpg	1018.52	J/mol×K	993.85	Joback Method
cpg	1031.03	J/mol×K	1030.01	Joback Method
cpg	1042.19	J/mol×K	1066.18	Joback Method
cpg	1052.04	J/mol×K	1102.35	Joback Method
cpg	1060.58	J/mol×K	1138.51	Joback Method
cpg	1067.83	J/mol×K	1174.68	Joback Method
dvisc	0.0002168	Pa×s	604.24	Joback Method

dvisc	0.0001323	Pa×s	663.15	Joback Method
dvisc	0.0000875	Pa×s	722.05	Joback Method
dvisc	0.0000616	Pa×s	780.96	Joback Method
dvisc	0.0000455	Pa×s	839.87	Joback Method
dvisc	0.0000350	Pa×s	898.77	Joback Method
dvisc	0.0000278	Pa×s	957.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406587&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