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

Inchi: InChI=1S/C19H27BrO5/c1-3-4-12-24-18(21)8-6-5-7-9-19(22)25-14-15-10-11-16(20)13-17

InchiKey: KJCCDIHSCGONFA-UHFFFAOYSA-N

Formula: C19H27BrO5

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

Mol. weight [g/mol]: 415.32

Physical Properties

Property code	Value	Unit	Source
gf	-356.27	kJ/mol	Joback Method
hf	-817.39	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.795		Crippen Method
mcvol	293.060	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	911.92	K	Joback Method
tc	1124.61	K	Joback Method
tf	581.70	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.11	J/mol×K	911.92	Joback Method
cpg	941.79	J/mol×K	1089.16	Joback Method
cpg	933.06	J/mol×K	1053.71	Joback Method
cpg	923.14	J/mol×K	1018.26	Joback Method
cpg	912.01	J/mol×K	982.82	Joback Method
cpg	899.67	J/mol×K	947.37	Joback Method
cpg	949.34	J/mol×K	1124.61	Joback Method
dvisc	0.0000376	Pa×s	911.92	Joback Method

dvisc	0.0000471	Pa×s	856.88	Joback Method
dvisc	0.0000607	Pa×s	801.85	Joback Method
dvisc	0.0000812	Pa×s	746.81	Joback Method
dvisc	0.0001139	Pa×s	691.77	Joback Method
dvisc	0.0001694	Pa×s	636.74	Joback Method
dvisc	0.0002714	Pa×s	581.70	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=U406584&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