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

Inchi: InChI=1S/C19H27BrO5/c1-14(2)12-24-18(21)7-5-4-6-8-19(22)25-13-15-9-10-16(20)11-1

InchiKey: UTKHLSAVNFGCNK-UHFFFAOYSA-N

Formula: C19H27BrO5

SMILES: COc1cc(Br)ccc1COC(=O)CCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 415.32

Physical Properties

Property code	Value	Unit	Source
gf	-358.71	kJ/mol	Joback Method
hf	-822.67	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.651		Crippen Method
mcvol	293.060	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	911.48	K	Joback Method
tc	1125.70	K	Joback Method
tf	566.70	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.61	J/mol×K	911.48	Joback Method
cpg	900.24	J/mol×K	947.18	Joback Method
cpg	912.61	J/mol×K	982.89	Joback Method
cpg	923.74	J/mol×K	1018.59	Joback Method
cpg	933.63	J/mol×K	1054.29	Joback Method
cpg	942.30	J/mol×K	1090.00	Joback Method
cpg	949.77	J/mol×K	1125.70	Joback Method
dvisc	0.0002932	Pa×s	566.70	Joback Method

dvisc	0.0001740	Pa×s	624.16	Joback Method
dvisc	0.0001128	Pa×s	681.63	Joback Method
dvisc	0.0000782	Pa×s	739.09	Joback Method
dvisc	0.0000571	Pa×s	796.55	Joback Method
dvisc	0.0000436	Pa×s	854.02	Joback Method
dvisc	0.0000344	Pa×s	911.48	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=U406583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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