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

Inchi: InChI=1S/C17H23BrO5/c1-3-22-16(19)7-5-4-6-8-17(20)23-12-13-9-10-14(18)11-15(13)21

InchiKey: UMIJAWFVASLJFO-UHFFFAOYSA-N

Formula: C17H23BrO5

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

Mol. weight [g/mol]: 387.27

Physical Properties

Property code	Value	Unit	Source
gf	-373.11	kJ/mol	Joback Method
hf	-776.11	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.014		Crippen Method
mcvol	264.880	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	866.16	K	Joback Method
tc	1077.81	K	Joback Method
tf	559.16	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.17	J/mol×K	866.16	Joback Method
cpg	825.08	J/mol×K	1042.54	Joback Method
cpg	816.32	J/mol×K	1007.26	Joback Method
cpg	806.45	J/mol×K	971.99	Joback Method
cpg	795.47	J/mol×K	936.71	Joback Method
cpg	783.38	J/mol×K	901.44	Joback Method
cpg	832.75	J/mol×K	1077.81	Joback Method
dvisc	0.0000505	Pa×s	866.16	Joback Method

dvisc	0.0000627	Pa×s	814.99	Joback Method
dvisc	0.0000802	Pa×s	763.83	Joback Method
dvisc	0.0001062	Pa×s	712.66	Joback Method
dvisc	0.0001468	Pa×s	661.49	Joback Method
dvisc	0.0002143	Pa×s	610.33	Joback Method
dvisc	0.0003352	Pa×s	559.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406581&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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