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

Inchi: InChI=1S/C20H29BrO5/c1-3-4-8-13-25-19(22)9-6-5-7-10-20(23)26-15-16-11-12-17(21)14

InchiKey: YDPPAZMDOQLUID-UHFFFAOYSA-N

Formula: C20H29BrO5

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

Mol. weight [g/mol]: 429.35

Physical Properties

Property code	Value	Unit	Source
gf	-347.85	kJ/mol	Joback Method
hf	-838.03	kJ/mol	Joback Method
hfus	52.87	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.185		Crippen Method
mcvol	307.150	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2853.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tb	934.80	K	Joback Method
tc	1149.21	K	Joback Method
tf	592.97	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.09	J/mol×K	934.80	Joback Method
cpg	958.81	J/mol×K	970.53	Joback Method
cpg	971.24	J/mol×K	1006.27	Joback Method
cpg	982.40	J/mol×K	1042.00	Joback Method
cpg	992.29	J/mol×K	1077.74	Joback Method
cpg	1000.95	J/mol×K	1113.47	Joback Method
cpg	1008.37	J/mol×K	1149.21	Joback Method
dvisc	0.0002430	Pa×s	592.97	Joback Method

dvisc	0.0001499	Pa×s	649.94	Joback Method
dvisc	0.0000999	Pa×s	706.91	Joback Method
dvisc	0.0000708	Pa×s	763.88	Joback Method
dvisc	0.0000526	Pa×s	820.86	Joback Method
dvisc	0.0000406	Pa×s	877.83	Joback Method
dvisc	0.0000324	Pa×s	934.80	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=U406586&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