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

Inchi: InChI=1S/C22H33BrO5/c1-3-4-5-6-10-15-27-21(24)11-8-7-9-12-22(25)28-17-18-13-14-19

InchiKey: UEDYDKKZHQNWKK-UHFFFAOYSA-N

Formula: C22H33BrO5

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

Mol. weight [g/mol]: 457.40

Physical Properties

Property code	Value	Unit	Source
gf	-331.01	kJ/mol	Joback Method
hf	-879.31	kJ/mol	Joback Method
hfus	58.05	kJ/mol	Joback Method
hvap	95.32	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.965		Crippen Method
mcvol	335.330	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	980.56	K	Joback Method
tc	1201.09	K	Joback Method
tf	615.51	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.74	J/mol×K	980.56	Joback Method
cpg	1078.75	J/mol×K	1017.31	Joback Method
cpg	1091.32	J/mol×K	1054.07	Joback Method
cpg	1102.48	J/mol×K	1090.82	Joback Method
cpg	1112.23	J/mol×K	1127.58	Joback Method
cpg	1120.62	J/mol×K	1164.33	Joback Method
cpg	1127.66	J/mol×K	1201.09	Joback Method
dvisc	0.0001929	Pa×s	615.51	Joback Method

dvisc	0.0001164	Pa×s	676.35	Joback Method
dvisc	0.0000764	Pa×s	737.19	Joback Method
dvisc	0.0000534	Pa×s	798.03	Joback Method
dvisc	0.0000393	Pa×s	858.88	Joback Method
dvisc	0.0000301	Pa×s	919.72	Joback Method
dvisc	0.0000239	Pa×s	980.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406588&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