Phthalic acid, 5-bromo-2-methoxybenzyl tridecyl ester

Inchi: InChI=1S/C29H39BrO5/c1-3-4-5-6-7-8-9-10-11-12-15-20-34-28(31)25-16-13-14-17-26(25

InchiKey: KLGMLNNFHGLAMD-UHFFFAOYSA-N

Formula: C29H39BrO5

SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 547.52

Physical Properties

Property code	Value	Unit	Source
gf	-169.29	kJ/mol	Joback Method
hf	-798.73	kJ/mol	Joback Method
hfus	69.83	kJ/mol	Joback Method
hvap	113.84	kJ/mol	Joback Method
log10ws	-10.37		Crippen Method
logp	8.282		Crippen Method
mcvol	410.200	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	3701.00		NIST Webbook
rinpol	3701.00		NIST Webbook
tb	1172.38	K	Joback Method
tc	1441.68	K	Joback Method
tf	733.34	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.74	J/mol×K	1172.38	Joback Method
cpg	1385.57	J/mol×K	1217.26	Joback Method
cpg	1394.28	J/mol×K	1262.15	Joback Method
cpg	1400.96	J/mol×K	1307.03	Joback Method
cpg	1405.71	J/mol×K	1351.91	Joback Method
cpg	1408.60	J/mol×K	1396.79	Joback Method
cpg	1409.72	J/mol×K	1441.68	Joback Method
dvisc	0.0000688	Pa×s	733.34	Joback Method

dvisc	0.0000415	Pa×s	806.51	Joback Method
dvisc	0.0000272	Pa×s	879.69	Joback Method
dvisc	0.0000190	Pa×s	952.86	Joback Method
dvisc	0.0000140	Pa×s	1026.03	Joback Method
dvisc	0.0000107	Pa×s	1099.21	Joback Method
dvisc	0.0000085	Pa×s	1172.38	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=U382875&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