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

Inchi: InChI=1S/C23H27BrO5/c1-3-4-5-6-9-14-28-22(25)19-10-7-8-11-20(19)23(26)29-16-17-15

InchiKey: UKBJSLYDLFRGAF-UHFFFAOYSA-N

Formula: C23H27BrO5

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

Mol. weight [g/mol]: 463.36

Physical Properties

Property code	Value	Unit	Source
gf	-219.81	kJ/mol	Joback Method
hf	-674.89	kJ/mol	Joback Method
hfus	54.29	kJ/mol	Joback Method
hvap	100.49	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	5.942		Crippen Method
mcvol	325.660	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	1035.10	K	Joback Method
tc	1271.69	K	Joback Method
tf	665.72	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.55	J/mol×K	1035.10	Joback Method
cpg	1053.80	J/mol×K	1232.26	Joback Method
cpg	1048.72	J/mol×K	1192.83	Joback Method
cpg	1042.19	J/mol×K	1153.40	Joback Method
cpg	1034.17	J/mol×K	1113.96	Joback Method
cpg	1024.63	J/mol×K	1074.53	Joback Method
cpg	1057.47	J/mol×K	1271.69	Joback Method
dvisc	0.0000218	Pa×s	1035.10	Joback Method

dvisc	0.0000271	Pa×s	973.54	Joback Method
dvisc	0.0000346	Pa×s	911.97	Joback Method
dvisc	0.0000458	Pa×s	850.41	Joback Method
dvisc	0.0000634	Pa×s	788.85	Joback Method
dvisc	0.0000926	Pa×s	727.28	Joback Method
dvisc	0.0001451	Pa×s	665.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382869&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