

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

Inchi:	InChI=1S/C28H37BrO5/c1-3-4-5-6-7-8-9-10-11-14-19-33-27(30)24-15-12-13-16-25(24)2
InchiKey:	POEKKWAXDORGRL-UHFFFAOYSA-N
Formula:	C28H37BrO5
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]:	533.49

Physical Properties

Property code	Value	Unit	Source
gf	-177.71	kJ/mol	Joback Method
hf	-778.09	kJ/mol	Joback Method
hfus	67.24	kJ/mol	Joback Method
hvap	111.62	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	7.892		Crippen Method
mvol	396.110	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	3600.00		NIST Webbook
rinpol	3600.00		NIST Webbook
tb	1149.50	K	Joback Method
tc	1410.23	K	Joback Method
tf	722.07	K	Joback Method
vc	1.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.89	J/molxK	1149.50	Joback Method
cpg	1324.77	J/molxK	1192.95	Joback Method
cpg	1333.66	J/molxK	1236.41	Joback Method
cpg	1340.64	J/molxK	1279.86	Joback Method
cpg	1345.79	J/molxK	1323.32	Joback Method
cpg	1349.17	J/molxK	1366.77	Joback Method
cpg	1350.87	J/molxK	1410.23	Joback Method
dvisc	0.0000784	Paxs	722.07	Joback Method

dvisc	0.0000476	Paxs	793.31	Joback Method
dvisc	0.0000314	Paxs	864.55	Joback Method
dvisc	0.0000221	Paxs	935.79	Joback Method
dvisc	0.0000163	Paxs	1007.02	Joback Method
dvisc	0.0000126	Paxs	1078.26	Joback Method
dvisc	0.0000100	Paxs	1149.50	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=U382874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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