Phthalic acid, 2-(3-bromophenyl)ethyl decyl ester

Inchi: InChI=1S/C26H33BrO4/c1-2-3-4-5-6-7-8-11-18-30-25(28)23-15-9-10-16-24(23)26(29)31-

InchiKey: XWBNDGAJBJXJHQ-UHFFFAOYSA-N

Formula: C26H33BrO4

SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 489.44

Physical Properties

Property code	Value	Unit	Source
gf	-79.92	kJ/mol	Joback Method
hf	-593.12	kJ/mol	Joback Method
hfus	61.26	kJ/mol	Joback Method
hvap	104.09	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.146		Crippen Method
mcvol	362.060	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	3387.00		NIST Webbook
rinpol	3387.00		NIST Webbook
tb	1076.34	K	Joback Method
tc	1318.10	K	Joback Method
tf	664.78	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.95	J/mol×K	1076.34	Joback Method
cpg	1182.65	J/mol×K	1116.63	Joback Method
cpg	1193.92	J/mol×K	1156.93	Joback Method
cpg	1203.83	J/mol×K	1197.22	Joback Method
cpg	1212.47	J/mol×K	1237.51	Joback Method
cpg	1219.92	J/mol×K	1277.80	Joback Method
cpg	1226.26	J/mol×K	1318.10	Joback Method
dvisc	0.0001565	Pa×s	664.78	Joback Method

dvisc	0.0000924	Pa×s	733.37	Joback Method
dvisc	0.0000597	Pa×s	801.97	Joback Method
dvisc	0.0000413	Pa×s	870.56	Joback Method
dvisc	0.0000302	Pa×s	939.15	Joback Method
dvisc	0.0000230	Pa×s	1007.75	Joback Method
dvisc	0.0000182	Pa×s	1076.34	Joback Method

Sources

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=U378029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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