Phthalic acid, 2-(4-bromophenoxy)ethyl decyl ester

Inchi: InChI=1S/C26H33BrO5/c1-2-3-4-5-6-7-8-11-18-31-25(28)23-12-9-10-13-24(23)26(29)32-

InchiKey: HEZHFQSXHGLOLG-UHFFFAOYSA-N

Formula: C26H33BrO5

SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 505.44

Physical Properties

Property code	Value	Unit	Source
gf	-184.92	kJ/mol	Joback Method
hf	-725.34	kJ/mol	Joback Method
hfus	62.45	kJ/mol	Joback Method
hvap	106.50	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	6.982		Crippen Method
mcvol	367.930	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	3434.00		NIST Webbook
rinpol	3434.00		NIST Webbook
tb	1098.76	K	Joback Method
tc	1345.20	K	Joback Method
tf	687.01	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.57	J/mol×K	1098.76	Joback Method
cpg	1234.50	J/mol×K	1304.12	Joback Method
cpg	1229.66	J/mol×K	1263.05	Joback Method
cpg	1223.31	J/mol×K	1221.98	Joback Method
cpg	1215.39	J/mol×K	1180.91	Joback Method
cpg	1205.83	J/mol×K	1139.83	Joback Method
cpg	1237.89	J/mol×K	1345.20	Joback Method
dvisc	0.0000133	Pa×s	1098.76	Joback Method

dvisc	0.0000168	Pa×s	1030.13	Joback Method
dvisc	0.0000219	Pa×s	961.51	Joback Method
dvisc	0.0000299	Pa×s	892.88	Joback Method
dvisc	0.0000428	Pa×s	824.26	Joback Method
dvisc	0.0000656	Pa×s	755.64	Joback Method
dvisc	0.0001094	Pa×s	687.01	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=U382899&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