

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

Inchi:	InChI=1S/C26H33BrO4/c1-2-3-4-5-6-7-8-13-19-30-25(28)22-15-10-11-16-23(22)26(29)3
InchiKey:	HYDMPRCLBJFDY-UHFFFAOYSA-N
Formula:	C26H33BrO4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1Br
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
mvol	362.060	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook
tb	1076.34	K	Joback Method
tc	1318.10	K	Joback Method
tf	664.78	K	Joback Method
vc	1.385	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000924	Paxs	733.37	Joback Method
dvisc	0.0000597	Paxs	801.97	Joback Method
dvisc	0.0000413	Paxs	870.56	Joback Method
dvisc	0.0000302	Paxs	939.15	Joback Method
dvisc	0.0000230	Paxs	1007.75	Joback Method
dvisc	0.0000182	Paxs	1076.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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