Sebacic acid, 2-(4-bromophenoxy)ethyl hexyl ester

Inchi: InChI=1S/C24H37BrO5/c1-2-3-4-11-18-29-23(26)12-9-7-5-6-8-10-13-24(27)30-20-19-28-
InchiKey: ISWGODUQEDMNCX-UHFFFAOYSA-N
Formula: C24H37BrO5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 485.45

Physical Properties

Property code	Value	Unit	Source
gf	-304.54	kJ/mol	Joback Method
hf	-909.12	kJ/mol	Joback Method
hfus	63.61	kJ/mol	Joback Method
hvap	99.11	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.615		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	3293.00		NIST Webbook
rinpol	3293.00		NIST Webbook
tb	1021.34	K	Joback Method
tc	1250.81	K	Joback Method
tf	625.53	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.35	J/mol×K	1021.34	Joback Method
cpg	1201.83	J/mol×K	1059.58	Joback Method
cpg	1214.72	J/mol×K	1097.83	Joback Method
cpg	1226.06	J/mol×K	1136.07	Joback Method
cpg	1235.90	J/mol×K	1174.32	Joback Method
cpg	1244.27	J/mol×K	1212.56	Joback Method
cpg	1251.21	J/mol×K	1250.81	Joback Method
dvisc	0.0001678	Pa×s	625.53	Joback Method

dvisc	0.0000955	Pa×s	691.50	Joback Method
dvisc	0.0000600	Pa×s	757.47	Joback Method
dvisc	0.0000406	Pa×s	823.43	Joback Method
dvisc	0.0000291	Pa×s	889.40	Joback Method
dvisc	0.0000218	Pa×s	955.37	Joback Method
dvisc	0.0000170	Pa×s	1021.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380598&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

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