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

Inchi: InChI=1S/C20H29BrO5/c1-2-24-19(22)9-7-5-3-4-6-8-10-20(23)26-16-15-25-18-13-11-17(

InchiKey: STOVXNLCODTLNQ-UHFFFAOYSA-N

Formula: C20H29BrO5

SMILES: CCOC(=O)CCCCCCCCC(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 429.35

Physical Properties

Property code	Value	Unit	Source
gf	-338.22	kJ/mol	Joback Method
hf	-826.56	kJ/mol	Joback Method
hfus	53.25	kJ/mol	Joback Method
hvap	90.21	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.055		Crippen Method
mcvol	307.150	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	929.82	K	Joback Method
tc	1143.30	K	Joback Method
tf	580.45	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.13	J/mol×K	929.82	Joback Method
cpg	1002.81	J/mol×K	1107.72	Joback Method
cpg	993.92	J/mol×K	1072.14	Joback Method
cpg	983.83	J/mol×K	1036.56	Joback Method
cpg	972.52	J/mol×K	1000.98	Joback Method
cpg	959.96	J/mol×K	965.40	Joback Method
cpg	1010.51	J/mol×K	1143.30	Joback Method
dvisc	0.0000317	Pa×s	929.82	Joback Method

dvisc	0.0000403	Pa×s	871.59	Joback Method
dvisc	0.0000529	Pa×s	813.36	Joback Method
dvisc	0.0000725	Pa×s	755.13	Joback Method
dvisc	0.0001046	Pa×s	696.91	Joback Method
dvisc	0.0001615	Pa×s	638.68	Joback Method
dvisc	0.0002721	Pa×s	580.45	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=U380594&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