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

Inchi: InChI=1S/C21H31BrO5/c1-2-15-26-20(23)9-7-5-3-4-6-8-10-21(24)27-17-16-25-19-13-11-
InchiKey: SFUYCLVFQIBUCJ-UHFFFAOYSA-N
Formula: C21H31BrO5
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 443.37

Physical Properties

Property code	Value	Unit	Source
gf	-329.80	kJ/mol	Joback Method
hf	-847.20	kJ/mol	Joback Method
hfus	55.84	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.445		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	952.70	K	Joback Method
tc	1168.72	K	Joback Method
tf	591.72	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.68	J/mol×K	952.70	Joback Method
cpg	1062.54	J/mol×K	1132.72	Joback Method
cpg	1053.73	J/mol×K	1096.71	Joback Method
cpg	1043.67	J/mol×K	1060.71	Joback Method
cpg	1032.32	J/mol×K	1024.71	Joback Method
cpg	1019.67	J/mol×K	988.70	Joback Method
cpg	1070.12	J/mol×K	1168.72	Joback Method
dvisc	0.0000272	Pa×s	952.70	Joback Method

dvisc	0.0000347	Pa×s	892.54	Joback Method
dvisc	0.0000457	Pa×s	832.37	Joback Method
dvisc	0.0000629	Pa×s	772.21	Joback Method
dvisc	0.0000914	Pa×s	712.05	Joback Method
dvisc	0.0001422	Pa×s	651.88	Joback Method
dvisc	0.0002421	Pa×s	591.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380595&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