Sebacic acid, 4-phenoxybenzyl pentyl ester

Inchi: InChI=1S/C28H38O5/c1-2-3-13-22-31-27(29)16-11-6-4-5-7-12-17-28(30)32-23-24-18-20
InchiKey: LNTRJDNTBAOIRA-UHFFFAOYSA-N
Formula: C28H38O5
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 454.60

Physical Properties

Property code	Value	Unit	Source
gf	-172.77	kJ/mol	Joback Method
hf	-781.48	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	103.86	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.376		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	3448.00		NIST Webbook
rinpol	3448.00		NIST Webbook
tb	1073.38	K	Joback Method
tc	1314.79	K	Joback Method
tf	637.23	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.96	J/mol×K	1073.38	Joback Method
cpg	1300.49	J/mol×K	1113.61	Joback Method
cpg	1312.16	J/mol×K	1153.85	Joback Method
cpg	1322.05	J/mol×K	1194.08	Joback Method
cpg	1330.22	J/mol×K	1234.32	Joback Method
cpg	1336.74	J/mol×K	1274.55	Joback Method
cpg	1341.67	J/mol×K	1314.79	Joback Method
dvisc	0.0001460	Pa×s	637.23	Joback Method

dvisc	0.0000790	Pa×s	709.92	Joback Method
dvisc	0.0000479	Pa×s	782.61	Joback Method
dvisc	0.0000316	Pa×s	855.30	Joback Method
dvisc	0.0000223	Pa×s	928.00	Joback Method
dvisc	0.0000165	Pa×s	1000.69	Joback Method
dvisc	0.0000128	Pa×s	1073.38	Joback Method

Sources

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=U355040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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