Sebacic acid, ethyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C25H32O5/c1-2-28-24(26)14-10-5-3-4-6-11-15-25(27)29-20-21-16-18-23(19-1
InchiKey: AQOUIRFQIQVGMH-UHFFFAOYSA-N
Formula: C25H32O5
SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-198.03	kJ/mol	Joback Method
hf	-719.56	kJ/mol	Joback Method
hfus	54.96	kJ/mol	Joback Method
hvap	97.18	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.206		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	3140.00		NIST Webbook
rinpol	3140.00		NIST Webbook
tb	1004.74	K	Joback Method
tc	1232.07	K	Joback Method
tf	603.42	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.35	J/mol×K	1004.74	Joback Method
cpg	1156.40	J/mol×K	1194.18	Joback Method
cpg	1149.00	J/mol×K	1156.29	Joback Method
cpg	1140.15	J/mol×K	1118.41	Joback Method
cpg	1129.78	J/mol×K	1080.52	Joback Method
cpg	1117.86	J/mol×K	1042.63	Joback Method
cpg	1162.37	J/mol×K	1232.07	Joback Method
dvisc	0.0000203	Pa×s	1004.74	Joback Method

dvisc	0.0000260	Pa×s	937.85	Joback Method
dvisc	0.0000348	Pa×s	870.97	Joback Method
dvisc	0.0000488	Pa×s	804.08	Joback Method
dvisc	0.0000727	Pa×s	737.19	Joback Method
dvisc	0.0001174	Pa×s	670.31	Joback Method
dvisc	0.0002109	Pa×s	603.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355036&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