Sebacic acid, di(2-phenoxyethyl) ester

Inchi: InChI=1S/C26H34O6/c27-25(31-21-19-29-23-13-7-5-8-14-23)17-11-3-1-2-4-12-18-26(28
InchiKey: CCOHSRRJVBDUOH-UHFFFAOYSA-N
Formula: C26H34O6
SMILES: O=C(CCCCCCCCC(=O)OCCOc1ccccc1)OCCOc1ccccc1
Mol. weight [g/mol]: 442.54

Physical Properties

Property code	Value	Unit	Source
gf	-284.98	kJ/mol	Joback Method
hf	-860.95	kJ/mol	Joback Method
hfus	59.13	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.352		Crippen Method
mcvol	356.300	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1045.06	K	Joback Method
tc	1279.45	K	Joback Method
tf	624.40	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.41	J/mol×K	1045.06	Joback Method
cpg	1204.88	J/mol×K	1084.13	Joback Method
cpg	1215.49	J/mol×K	1123.19	Joback Method
cpg	1224.28	J/mol×K	1162.26	Joback Method
cpg	1231.30	J/mol×K	1201.32	Joback Method
cpg	1236.59	J/mol×K	1240.39	Joback Method
cpg	1240.18	J/mol×K	1279.45	Joback Method
dvisc	0.0001446	Pa×s	624.40	Joback Method

dvisc	0.0000781	Pa×s	694.51	Joback Method
dvisc	0.0000473	Pa×s	764.62	Joback Method
dvisc	0.0000311	Pa×s	834.73	Joback Method
dvisc	0.0000219	Pa×s	904.84	Joback Method
dvisc	0.0000162	Pa×s	974.95	Joback Method
dvisc	0.0000124	Pa×s	1045.06	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380789&Units=SI

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