Sebacic acid, decyl 2-phenoxyethyl ester

Inchi: InChI=1S/C28H46O5/c1-2-3-4-5-6-9-12-18-23-32-27(29)21-16-10-7-8-11-17-22-28(30)33
InchiKey: AETIFEAXOVXOHJ-UHFFFAOYSA-N
Formula: C28H46O5
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-275.55	kJ/mol	Joback Method
hf	-1006.54	kJ/mol	Joback Method
hfus	69.08	kJ/mol	Joback Method
hvap	100.92	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.413		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	816.33	kPa	Joback Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook
tb	1041.72	K	Joback Method
tc	1283.59	K	Joback Method
tf	598.29	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.19	J/mol×K	1041.72	Joback Method
cpg	1416.67	J/mol×K	1082.03	Joback Method
cpg	1432.12	J/mol×K	1122.34	Joback Method
cpg	1445.60	J/mol×K	1162.66	Joback Method
cpg	1457.19	J/mol×K	1202.97	Joback Method
cpg	1466.94	J/mol×K	1243.28	Joback Method
cpg	1474.92	J/mol×K	1283.59	Joback Method
dvisc	0.0001833	Pa×s	598.29	Joback Method

dvisc	0.0000905	Pa×s	672.19	Joback Method
dvisc	0.0000514	Pa×s	746.10	Joback Method
dvisc	0.0000323	Pa×s	820.00	Joback Method
dvisc	0.0000220	Pa×s	893.91	Joback Method
dvisc	0.0000158	Pa×s	967.81	Joback Method
dvisc	0.0000119	Pa×s	1041.72	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=U380788&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