Sebacic acid, octyl 2-phenoxyethyl ester

Inchi: InChI=1S/C26H42O5/c1-2-3-4-5-10-16-21-30-25(27)19-14-8-6-7-9-15-20-26(28)31-23-22
InchiKey: SDQKTGARNVTMFF-UHFFFAOYSA-N
Formula: C26H42O5
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 434.61

Physical Properties

Property code	Value	Unit	Source
gf	-292.39	kJ/mol	Joback Method
hf	-965.26	kJ/mol	Joback Method
hfus	63.90	kJ/mol	Joback Method
hvap	96.47	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.633		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	913.84	kPa	Joback Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
tb	995.96	K	Joback Method
tc	1221.12	K	Joback Method
tf	575.75	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.80	J/mol×K	995.96	Joback Method
cpg	1290.75	J/mol×K	1033.49	Joback Method
cpg	1305.98	J/mol×K	1071.01	Joback Method
cpg	1319.53	J/mol×K	1108.54	Joback Method
cpg	1331.43	J/mol×K	1146.07	Joback Method
cpg	1341.74	J/mol×K	1183.60	Joback Method
cpg	1350.51	J/mol×K	1221.12	Joback Method
dvisc	0.0002376	Pa×s	575.75	Joback Method

dvisc	0.0001195	Pa×s	645.78	Joback Method
dvisc	0.0000687	Pa×s	715.82	Joback Method
dvisc	0.0000436	Pa×s	785.86	Joback Method
dvisc	0.0000298	Pa×s	855.89	Joback Method
dvisc	0.0000216	Pa×s	925.92	Joback Method
dvisc	0.0000164	Pa×s	995.96	Joback Method

Sources

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=U380786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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