Sebacic acid, isobutyl 2-phenoxyethyl ester

Inchi: InChI=1S/C22H34O5/c1-19(2)18-27-22(24)15-11-6-4-3-5-10-14-21(23)26-17-16-25-20-1
InchiKey: RCHRYLQSIBPXTK-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-328.51	kJ/mol	Joback Method
hf	-887.98	kJ/mol	Joback Method
hfus	50.02	kJ/mol	Joback Method
hvap	87.18	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.929		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	2744.00		NIST Webbook
rinpol	2744.00		NIST Webbook
tb	904.00	K	Joback Method
tc	1109.92	K	Joback Method
tf	515.67	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.12	J/mol×K	904.00	Joback Method
cpg	1044.26	J/mol×K	938.32	Joback Method
cpg	1059.05	J/mol×K	972.64	Joback Method
cpg	1072.50	J/mol×K	1006.96	Joback Method
cpg	1084.65	J/mol×K	1041.28	Joback Method
cpg	1095.51	J/mol×K	1075.60	Joback Method
cpg	1105.10	J/mol×K	1109.92	Joback Method
dvisc	0.0004354	Pa×s	515.67	Joback Method

dvisc	0.0002127	Pa×s	580.39	Joback Method
dvisc	0.0001200	Pa×s	645.11	Joback Method
dvisc	0.0000751	Pa×s	709.83	Joback Method
dvisc	0.0000509	Pa×s	774.56	Joback Method
dvisc	0.0000366	Pa×s	839.28	Joback Method
dvisc	0.0000276	Pa×s	904.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380781&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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