Sebacic acid, 4-formylphenyl octyl ester

Inchi: InChI=1S/C25H38O5/c1-2-3-4-5-10-13-20-29-24(27)14-11-8-6-7-9-12-15-25(28)30-23-18
InchiKey: WGXXYWJCDLDGFT-UHFFFAOYSA-N
Formula: C25H38O5
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-304.96	kJ/mol	Joback Method
hf	-909.45	kJ/mol	Joback Method
hfus	62.02	kJ/mol	Joback Method
hvap	99.21	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.429		Crippen Method
mcvol	355.800	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	3321.00		NIST Webbook
rinpol	3321.00		NIST Webbook
tb	1004.30	K	Joback Method
tc	1230.41	K	Joback Method
tf	596.77	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.22	J/mol×K	1004.30	Joback Method
cpg	1210.68	J/mol×K	1041.99	Joback Method
cpg	1224.60	J/mol×K	1079.67	Joback Method
cpg	1237.02	J/mol×K	1117.36	Joback Method
cpg	1248.01	J/mol×K	1155.04	Joback Method
cpg	1257.60	J/mol×K	1192.73	Joback Method
cpg	1265.86	J/mol×K	1230.41	Joback Method
dvisc	0.0003203	Pa×s	596.77	Joback Method

dvisc	0.0001736	Pa×s	664.69	Joback Method
dvisc	0.0001054	Pa×s	732.61	Joback Method
dvisc	0.0000697	Pa×s	800.53	Joback Method
dvisc	0.0000491	Pa×s	868.46	Joback Method
dvisc	0.0000365	Pa×s	936.38	Joback Method
dvisc	0.0000282	Pa×s	1004.30	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=U354892&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