Sebacic acid, hexyl 4-methylbenzyl ester

Inchi: InChI=1S/C24H38O4/c1-3-4-5-12-19-27-23(25)13-10-8-6-7-9-11-14-24(26)28-20-22-17-1
InchiKey: SXFYVNJKXAEJMS-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(C)cc1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.86	kJ/mol	Joback Method
hf	-803.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	90.27	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.283		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook
tb	932.76	K	Joback Method
tc	1142.45	K	Joback Method
tf	543.50	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.44	J/mol×K	932.76	Joback Method
cpg	1136.46	J/mol×K	967.71	Joback Method
cpg	1152.13	J/mol×K	1002.66	Joback Method
cpg	1166.46	J/mol×K	1037.60	Joback Method
cpg	1179.51	J/mol×K	1072.55	Joback Method
cpg	1191.30	J/mol×K	1107.50	Joback Method
cpg	1201.88	J/mol×K	1142.45	Joback Method
dvisc	0.0003848	Pa×s	543.50	Joback Method

dvisc	0.0002018	Pa×s	608.38	Joback Method
dvisc	0.0001199	Pa×s	673.25	Joback Method
dvisc	0.0000780	Pa×s	738.13	Joback Method
dvisc	0.0000544	Pa×s	803.01	Joback Method
dvisc	0.0000401	Pa×s	867.88	Joback Method
dvisc	0.0000308	Pa×s	932.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380706&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

Latest version available from:
https://www.chemeo.com/cid/84-067-5/Sebacic-acid-hexyl-4-methylbenzyl-ester.pdf
Generated by Cheméo on 2024-10-12 02:14:40.026997968 +0000 UTC m=+3280142.663967217.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.