Dibenzyl sebacate

Other names: Decanedioic acid, bis(phenylmethyl) ester
Sebacic acid, dibenzyl ester
Inchi: InChI=1S/C24H30O4/c25-23(27-19-21-13-7-5-8-14-21)17-11-3-1-2-4-12-18-24(26)28-20
InchiKey: DVLXEVMGHXWBOZ-UHFFFAOYSA-N
Formula: C24H30O4
SMILES: O=C(CCCCCCCCC(=O)OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 382.49
CAS: 140-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-91.82	kJ/mol	Joback Method
hf	-555.23	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	91.88	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.594		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
tb	954.46	K	Joback Method
tc	1176.26	K	Joback Method
tf	557.40	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.14	J/mol×K	1102.33	Joback Method
cpg	1086.03	J/mol×K	1176.26	Joback Method
cpg	1077.64	J/mol×K	1139.30	Joback Method
cpg	1017.74	J/mol×K	954.46	Joback Method
cpg	1032.32	J/mol×K	991.43	Joback Method
cpg	1045.53	J/mol×K	1028.39	Joback Method
cpg	1057.45	J/mol×K	1065.36	Joback Method

dvisc	0.0000311	Pa×s	954.46	Joback Method
dvisc	0.0000549	Pa×s	822.11	Joback Method
dvisc	0.0000405	Pa×s	888.28	Joback Method
dvisc	0.0003856	Pa×s	557.40	Joback Method
dvisc	0.0002028	Pa×s	623.58	Joback Method
dvisc	0.0001207	Pa×s	689.75	Joback Method
dvisc	0.0000787	Pa×s	755.93	Joback Method
hvapt	121.00	kJ/mol	402.50	NIST Webbook
hvapt	112.20	kJ/mol	434.00	NIST Webbook
hvapt	114.30	kJ/mol	459.00	NIST Webbook

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=C140249&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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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