Sebacic acid, decyl 4-methoxybenzyl ester

Inchi: InChI=1S/C28H46O5/c1-3-4-5-6-7-10-13-16-23-32-27(29)17-14-11-8-9-12-15-18-28(30)3
InchiKey: RPCNZONJOOTMEX-UHFFFAOYSA-N
Formula: C28H46O5
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-285.18	kJ/mol	Joback Method
hf	-1018.01	kJ/mol	Joback Method
hfus	68.69	kJ/mol	Joback Method
hvap	101.58	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.543		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	3529.00		NIST Webbook
rinpol	3529.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1290.03	K	Joback Method
tf	610.81	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.39	J/mol×K	1046.70	Joback Method
cpg	1464.35	J/mol×K	1249.48	Joback Method
cpg	1455.12	J/mol×K	1208.92	Joback Method
cpg	1443.96	J/mol×K	1168.37	Joback Method
cpg	1430.83	J/mol×K	1127.81	Joback Method
cpg	1415.66	J/mol×K	1087.26	Joback Method
cpg	1471.71	J/mol×K	1290.03	Joback Method
dvisc	0.0000123	Pa×s	1046.70	Joback Method

dvisc	0.0000161	Pa×s	974.05	Joback Method
dvisc	0.0000220	Pa×s	901.40	Joback Method
dvisc	0.0000318	Pa×s	828.75	Joback Method
dvisc	0.0000493	Pa×s	756.11	Joback Method
dvisc	0.0000840	Pa×s	683.46	Joback Method
dvisc	0.0001623	Pa×s	610.81	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=U354369&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

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