

Sebacic acid, 2-methylbenzyl undecyl ester

Inchi: InChI=1S/C29H48O4/c1-3-4-5-6-7-8-11-14-19-24-32-28(30)22-15-12-9-10-13-16-23-29(3)
InchiKey: ZSRLTTQLZCKTLH-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-171.76	kJ/mol	Joback Method
hf	-906.43	kJ/mol	Joback Method
hfus	70.09	kJ/mol	Joback Method
hvap	101.40	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.233		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	774.18	kPa	Joback Method
rinpol	3240.00		NIST Webbook
rinpol	3240.00		NIST Webbook
tb	1047.16	K	Joback Method
tc	1291.10	K	Joback Method
tf	599.85	K	Joback Method
vc	1.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.07	J/molxK	1047.16	Joback Method
cpg	1451.70	J/molxK	1087.82	Joback Method
cpg	1468.40	J/molxK	1128.47	Joback Method
cpg	1483.25	J/molxK	1169.13	Joback Method
cpg	1496.34	J/molxK	1209.79	Joback Method
cpg	1507.75	J/molxK	1250.44	Joback Method
cpg	1517.56	J/molxK	1291.10	Joback Method
dvisc	0.0002083	Paxs	599.85	Joback Method

dvisc	0.0001042	Paxs	674.40	Joback Method
dvisc	0.0000598	Paxs	748.95	Joback Method
dvisc	0.0000380	Paxs	823.50	Joback Method
dvisc	0.0000260	Paxs	898.06	Joback Method
dvisc	0.0000189	Paxs	972.61	Joback Method
dvisc	0.0000143	Paxs	1047.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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