

Sebacic acid, hexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C25H40O4/c1-2-3-4-14-21-28-24(26)19-12-7-5-6-8-13-20-25(27)29-22-15-18-2
InchiKey:	FOKNLCXBWODNGX-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-195.81	kJ/mol	Joback Method
hf	-812.40	kJ/mol	Joback Method
hfus	60.12	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.407		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3090.00		NIST Webbook
tb	950.66	K	Joback Method
tc	1163.88	K	Joback Method
tf	542.25	K	Joback Method
vc	1.375	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.85	J/molxK	950.66	Joback Method
cpg	1199.24	J/molxK	986.20	Joback Method
cpg	1215.22	J/molxK	1021.73	Joback Method
cpg	1229.82	J/molxK	1057.27	Joback Method
cpg	1243.10	J/molxK	1092.80	Joback Method
cpg	1255.10	J/molxK	1128.34	Joback Method
cpg	1265.88	J/molxK	1163.88	Joback Method
dvisc	0.0003943	Paxs	542.25	Joback Method
dvisc	0.0001945	Paxs	610.32	Joback Method

dvisc	0.0001106	Paxs	678.39	Joback Method
dvisc	0.0000697	Paxs	746.45	Joback Method
dvisc	0.0000475	Paxs	814.52	Joback Method
dvisc	0.0000343	Paxs	882.59	Joback Method
dvisc	0.0000259	Paxs	950.66	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354390&Units=SI

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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