

Sebacic acid, heptyl 2-methylbenzyl ester

Inchi:	InChI=1S/C25H40O4/c1-3-4-5-10-15-20-28-24(26)18-11-8-6-7-9-12-19-25(27)29-21-23-
InchiKey:	KXNABPRVOGBCSO-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCC(=O)CCCCCCCC(=O)OCc1cccc1C
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-205.44	kJ/mol	Joback Method
hf	-823.87	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.673		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2960.00		NIST Webbook
rinpol	2960.00		NIST Webbook
tb	955.64	K	Joback Method
tc	1169.97	K	Joback Method
tf	554.77	K	Joback Method
vc	1.375	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.32	J/molxK	955.64	Joback Method
cpg	1198.61	J/molxK	991.36	Joback Method
cpg	1214.46	J/molxK	1027.08	Joback Method
cpg	1228.89	J/molxK	1062.81	Joback Method
cpg	1241.97	J/molxK	1098.53	Joback Method
cpg	1253.73	J/molxK	1134.25	Joback Method
cpg	1264.21	J/molxK	1169.97	Joback Method
dvisc	0.0003423	Paxs	554.77	Joback Method

dvisc	0.0001777	Paxs	621.58	Joback Method
dvisc	0.0001048	Paxs	688.39	Joback Method
dvisc	0.0000678	Paxs	755.20	Joback Method
dvisc	0.0000471	Paxs	822.02	Joback Method
dvisc	0.0000346	Paxs	888.83	Joback Method
dvisc	0.0000265	Paxs	955.64	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=U380718&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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