

Sebacic acid, 2,3-dimethylphenyl heptyl ester

Inchi:	InChI=1S/C25H40O4/c1-4-5-6-11-14-20-28-24(26)18-12-9-7-8-10-13-19-25(27)29-23-17
InchiKey:	XTBIBCSSYGKCSM-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-215.07	kJ/mol	Joback Method
hf	-835.34	kJ/mol	Joback Method
hfus	59.34	kJ/mol	Joback Method
hvap	93.16	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.843		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	3034.00		NIST Webbook
rinpol	3034.00		NIST Webbook
tb	960.62	K	Joback Method
tc	1176.07	K	Joback Method
tf	567.29	K	Joback Method
vc	1.375	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.77	J/molxK	960.62	Joback Method
cpg	1252.28	J/molxK	1140.16	Joback Method
cpg	1240.78	J/molxK	1104.25	Joback Method
cpg	1227.92	J/molxK	1068.35	Joback Method
cpg	1213.65	J/molxK	1032.44	Joback Method
cpg	1197.95	J/molxK	996.53	Joback Method
cpg	1262.45	J/molxK	1176.07	Joback Method
dvisc	0.0000271	Paxs	960.62	Joback Method

dvisc	0.0000349	Paxs	895.06	Joback Method
dvisc	0.0000469	Paxs	829.51	Joback Method
dvisc	0.0000662	Paxs	763.95	Joback Method
dvisc	0.0000997	Paxs	698.40	Joback Method
dvisc	0.0001634	Paxs	632.84	Joback Method
dvisc	0.0003003	Paxs	567.29	Joback Method

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=U355210&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
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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