

Phthalic acid, 2,4,4-trimethylpentyl undecyl ester

Inchi:	InChI=1S/C27H44O4/c1-6-7-8-9-10-11-12-13-16-19-30-25(28)23-17-14-15-18-24(23)26(
InchiKey:	DEUFMHJGFLKSDJ-UHFFFAOYSA-N
Formula:	C27H44O4
SMILES:	CCCCCCCCCOC(=O)c1cccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	432.64

Physical Properties

Property code	Value	Unit	Source
gf	-188.20	kJ/mol	Joback Method
hf	-879.18	kJ/mol	Joback Method
hfus	53.98	kJ/mol	Joback Method
hvap	95.26	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.603		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2885.00		NIST Webbook
tb	997.73	K	Joback Method
tc	1221.62	K	Joback Method
tf	564.73	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.64	J/molxK	997.73	Joback Method
cpg	1324.38	J/molxK	1035.04	Joback Method
cpg	1340.63	J/molxK	1072.36	Joback Method
cpg	1355.47	J/molxK	1109.67	Joback Method
cpg	1368.98	J/molxK	1146.99	Joback Method
cpg	1381.24	J/molxK	1184.30	Joback Method
cpg	1392.33	J/molxK	1221.62	Joback Method
dvisc	0.0002587	Paxs	564.73	Joback Method
dvisc	0.0001195	Paxs	636.90	Joback Method

dvisc	0.0000646	Paxs	709.06	Joback Method
dvisc	0.0000391	Paxs	781.23	Joback Method
dvisc	0.0000258	Paxs	853.40	Joback Method
dvisc	0.0000181	Paxs	925.56	Joback Method
dvisc	0.0000134	Paxs	997.73	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=U377777&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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