

1,3-diundec-10'-enoylpropanediol

Inchi:	InChI=1S/C25H44O4/c1-3-5-7-9-11-13-15-17-20-24(26)28-22-19-23-29-25(27)21-18-16-
InchiKey:	CHJHMAIVZJVJQF-UHFFFAOYSA-N
Formula:	C25H44O4
SMILES:	C=CCCCCCCCC(=O)OCCOC(=O)CCCCCCCC=C
Mol. weight [g/mol]:	408.61

Physical Properties

Property code	Value	Unit	Source
gf	-132.54	kJ/mol	Joback Method
hf	-798.07	kJ/mol	Joback Method
hfus	63.52	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	2783.00		NIST Webbook
tb	917.34	K	Joback Method
tc	1124.73	K	Joback Method
tf	512.31	K	Joback Method
vc	1.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.68	J/molxK	917.34	Joback Method
cpg	1307.16	J/molxK	1090.16	Joback Method
cpg	1292.80	J/molxK	1055.60	Joback Method
cpg	1277.22	J/molxK	1021.03	Joback Method
cpg	1260.37	J/molxK	986.47	Joback Method
cpg	1242.21	J/molxK	951.90	Joback Method
cpg	1320.36	J/molxK	1124.73	Joback Method
dvisc	0.0000293	Paxs	917.34	Joback Method
dvisc	0.0000389	Paxs	849.83	Joback Method

dvisc	0.0000542	Paxs	782.33	Joback Method
dvisc	0.0000804	Paxs	714.82	Joback Method
dvisc	0.0001295	Paxs	647.32	Joback Method
dvisc	0.0002333	Paxs	579.81	Joback Method
dvisc	0.0004905	Paxs	512.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R391070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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