

1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl undecyl ester

Inchi: InChI=1S/C25H46O4/c1-5-7-8-9-10-11-12-13-16-19-28-24(26)21-17-14-15-18-22(21)25(26)24
InchiKey: XPAHPUCHQKQVJT-UHFFFAOYSA-N
Formula: C25H46O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-296.36	kJ/mol	Joback Method
hf	-1025.51	kJ/mol	Joback Method
hfus	51.94	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.845		Crippen Method
mvol	367.130	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	937.98	K	Joback Method
tc	1148.53	K	Joback Method
tf	488.97	K	Joback Method
vc	1.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.04	J/molxK	937.98	Joback Method
cpg	1365.35	J/molxK	1113.44	Joback Method
cpg	1352.21	J/molxK	1078.35	Joback Method
cpg	1337.44	J/molxK	1043.26	Joback Method
cpg	1321.01	J/molxK	1008.16	Joback Method
cpg	1302.89	J/molxK	973.07	Joback Method
cpg	1376.91	J/molxK	1148.53	Joback Method
dvisc	0.0000286	Paxs	937.98	Joback Method

dvisc	0.0000390	Paxs	863.14	Joback Method
dvisc	0.0000564	Paxs	788.31	Joback Method
dvisc	0.0000881	Paxs	713.47	Joback Method
dvisc	0.0001527	Paxs	638.64	Joback Method
dvisc	0.0003066	Paxs	563.81	Joback Method
dvisc	0.0007620	Paxs	488.97	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=U339448&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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