

1,2,4-Cyclohexanetricarboxylic acid, 2,2,4-trimethylpentyl ester

Inchi:	InChI=1S/C33H60O6/c1-22(2)16-31(7,8)19-37-28(34)25-13-14-26(29(35)38-20-32(9,10)
InchiKey:	ZVATUIQDXPRJFN-UHFFFAOYSA-N
Formula:	C33H60O6
SMILES:	CC(C)CC(C)(C)COC(=O)C1CCC(C(=O)OCC(C)(C)CC(C)C)C(C(=O)OCC(C)(C)CC(C)C)
Mol. weight [g/mol]:	552.83
CAS:	116401-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-464.55	kJ/mol	Joback Method
hf	-1487.30	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	111.28	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.865		Crippen Method
mcvol	487.290	ml/mol	McGowan Method
pc	616.34	kPa	Joback Method
tb	1182.51	K	Joback Method
tc	1465.81	K	Joback Method
tf	639.31	K	Joback Method
vc	1.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1842.19	J/molxK	1182.51	Joback Method
cpg	1859.21	J/molxK	1229.73	Joback Method
cpg	1873.74	J/molxK	1276.94	Joback Method
cpg	1886.00	J/molxK	1324.16	Joback Method
cpg	1896.22	J/molxK	1371.38	Joback Method
cpg	1904.63	J/molxK	1418.60	Joback Method
cpg	1911.45	J/molxK	1465.81	Joback Method
dvisc	0.0000936	Paxs	639.31	Joback Method
dvisc	0.0000356	Paxs	729.84	Joback Method

dvisc	0.0000167	Paxs	820.38	Joback Method
dvisc	0.0000092	Paxs	910.91	Joback Method
dvisc	0.0000056	Paxs	1001.44	Joback Method
dvisc	0.0000037	Paxs	1091.98	Joback Method
dvisc	0.0000026	Paxs	1182.51	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=C116401253&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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