

1,2-Cyclohexanedicarboxylic acid, heptyl pentadecyl ester

Inchi:	InChI=1S/C30H56O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-22-26-34-30(32)28-24-20-19-
InchiKey:	GPSCEVFREBAQSZ-UHFFFAOYSA-N
Formula:	C30H56O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC
Mol. weight [g/mol]:	480.76

Physical Properties

Property code	Value	Unit	Source
gf	-249.38	kJ/mol	Joback Method
hf	-1118.15	kJ/mol	Joback Method
hfus	71.94	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.941		Crippen Method
mvol	437.580	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	3345.00		NIST Webbook
rinpol	3345.00		NIST Webbook
tb	1053.26	K	Joback Method
tc	1304.73	K	Joback Method
tf	575.32	K	Joback Method
vc	1.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.51	J/molxK	1053.26	Joback Method
cpg	1625.68	J/molxK	1095.17	Joback Method
cpg	1644.32	J/molxK	1137.08	Joback Method
cpg	1660.52	J/molxK	1179.00	Joback Method
cpg	1674.38	J/molxK	1220.91	Joback Method
cpg	1685.97	J/molxK	1262.82	Joback Method
cpg	1695.39	J/molxK	1304.73	Joback Method
dvisc	0.0003062	Paxs	575.32	Joback Method

dvisc	0.0001386	Paxs	654.98	Joback Method
dvisc	0.0000745	Paxs	734.63	Joback Method
dvisc	0.0000452	Paxs	814.29	Joback Method
dvisc	0.0000300	Paxs	893.95	Joback Method
dvisc	0.0000213	Paxs	973.60	Joback Method
dvisc	0.0000159	Paxs	1053.26	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=U339543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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