

1,2-Cyclohexanedicarboxylic acid, hexyl pentadecyl ester

Inchi:	InChI=1S/C29H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-21-25-33-29(31)27-23-19-18-
InchiKey:	ZCTBNVXRGSJZOZ-UHFFFAOYSA-N
Formula:	C29H54O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	466.74

Physical Properties

Property code	Value	Unit	Source
gf	-257.80	kJ/mol	Joback Method
hf	-1097.51	kJ/mol	Joback Method
hfus	69.35	kJ/mol	Joback Method
hvap	98.58	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.551		Crippen Method
mvol	423.490	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	3255.00		NIST Webbook
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tb	1030.38	K	Joback Method
tc	1271.14	K	Joback Method
tf	564.05	K	Joback Method
vc	1.639	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.62	J/molxK	1030.38	Joback Method
cpg	1621.57	J/molxK	1231.01	Joback Method
cpg	1609.51	J/molxK	1190.88	Joback Method
cpg	1595.36	J/molxK	1150.76	Joback Method
cpg	1579.04	J/molxK	1110.63	Joback Method
cpg	1560.49	J/molxK	1070.51	Joback Method
cpg	1631.62	J/molxK	1271.14	Joback Method
dvisc	0.0000186	Paxs	1030.38	Joback Method

dvisc	0.0000249	Paxs	952.66	Joback Method
dvisc	0.0000350	Paxs	874.94	Joback Method
dvisc	0.0000526	Paxs	797.22	Joback Method
dvisc	0.0000862	Paxs	719.49	Joback Method
dvisc	0.0001595	Paxs	641.77	Joback Method
dvisc	0.0003496	Paxs	564.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339419&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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