

1,2-Cyclohexanedicarboxylic acid, dodecyl 4-octyl ester

Inchi:	InChI=1S/C28H52O4/c1-4-7-9-10-11-12-13-14-15-18-23-31-27(29)25-21-16-17-22-26(25)
InchiKey:	VTEPKWGXPKYERE-UHFFFAOYSA-N
Formula:	C28H52O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC
Mol. weight [g/mol]:	452.71

Physical Properties

Property code	Value	Unit	Source
gf	-268.66	kJ/mol	Joback Method
hf	-1082.15	kJ/mol	Joback Method
hfus	63.23	kJ/mol	Joback Method
hvap	95.97	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.159		Crippen Method
mvol	409.400	ml/mol	McGowan Method
pc	757.23	kPa	Joback Method
rinpol	2959.00		NIST Webbook
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tb	1007.06	K	Joback Method
tc	1237.11	K	Joback Method
tf	537.78	K	Joback Method
vc	1.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.18	J/molxK	1007.06	Joback Method
cpg	1495.60	J/molxK	1045.40	Joback Method
cpg	1513.90	J/molxK	1083.74	Joback Method
cpg	1530.14	J/molxK	1122.09	Joback Method
cpg	1544.39	J/molxK	1160.43	Joback Method
cpg	1556.70	J/molxK	1198.77	Joback Method
cpg	1567.14	J/molxK	1237.11	Joback Method
dvisc	0.0004472	Paxs	537.78	Joback Method

dvisc	0.0001912	Paxs	615.99	Joback Method
dvisc	0.0000990	Paxs	694.21	Joback Method
dvisc	0.0000586	Paxs	772.42	Joback Method
dvisc	0.0000382	Paxs	850.63	Joback Method
dvisc	0.0000267	Paxs	928.85	Joback Method
dvisc	0.0000198	Paxs	1007.06	Joback Method

Sources

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=U339527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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