

1,2-Cyclohexanedicarboxylic acid, heptadecyl methyl ester

Inchi:	InChI=1S/C26H48O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-30-26(28)24-21-18-
InchiKey:	JWGAUUILBBPDFE-UHFFFAOYSA-N
Formula:	C26H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCC1C(=O)OC
Mol. weight [g/mol]:	424.66

Physical Properties

Property code	Value	Unit	Source
gf	-283.06	kJ/mol	Joback Method
hf	-1035.59	kJ/mol	Joback Method
hfus	61.58	kJ/mol	Joback Method
hvap	91.90	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.380		Crippen Method
mvol	381.220	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	3040.00		NIST Webbook
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tb	961.74	K	Joback Method
tc	1178.14	K	Joback Method
tf	530.24	K	Joback Method
vc	1.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.18	J/molxK	961.74	Joback Method
cpg	1366.30	J/molxK	997.81	Joback Method
cpg	1384.59	J/molxK	1033.87	Joback Method
cpg	1401.10	J/molxK	1069.94	Joback Method
cpg	1415.87	J/molxK	1106.01	Joback Method
cpg	1428.94	J/molxK	1142.08	Joback Method
cpg	1440.35	J/molxK	1178.14	Joback Method
dvisc	0.0005127	Paxs	530.24	Joback Method

dvisc	0.0002399	Paxs	602.16	Joback Method
dvisc	0.0001320	Paxs	674.07	Joback Method
dvisc	0.0000815	Paxs	745.99	Joback Method
dvisc	0.0000548	Paxs	817.91	Joback Method
dvisc	0.0000393	Paxs	889.82	Joback Method
dvisc	0.0000296	Paxs	961.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339663&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
log_p:	Octanol/Water partition coefficient
m_cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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