

Adipic acid, 3-methylbutyl octadecyl ester

Inchi:	InChI=1S/C29H56O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-32-28(30)22-19
InchiKey:	VRNNYSINFXROKB-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	468.75

Physical Properties

Property code	Value	Unit	Source
gf	-276.98	kJ/mol	Joback Method
hf	-1136.77	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mvol	434.350	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	3206.00		NIST Webbook
rinpol	3206.00		NIST Webbook
tb	1015.06	K	Joback Method
tc	1265.21	K	Joback Method
tf	545.91	K	Joback Method
vc	1.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.99	J/molxK	1015.06	Joback Method
cpg	1563.19	J/molxK	1056.75	Joback Method
cpg	1584.14	J/molxK	1098.44	Joback Method
cpg	1602.93	J/molxK	1140.13	Joback Method
cpg	1619.67	J/molxK	1181.83	Joback Method
cpg	1634.42	J/molxK	1223.52	Joback Method
cpg	1647.29	J/molxK	1265.21	Joback Method
dvisc	0.0003091	Paxs	545.91	Joback Method

dvisc	0.0001288	Paxs	624.10	Joback Method
dvisc	0.0000652	Paxs	702.29	Joback Method
dvisc	0.0000378	Paxs	780.49	Joback Method
dvisc	0.0000242	Paxs	858.68	Joback Method
dvisc	0.0000167	Paxs	936.87	Joback Method
dvisc	0.0000122	Paxs	1015.06	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=U353519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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