

Adipic acid, heptadecyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C29H56O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-32-28(30)23-20-
InchiKey:	ACDHVGDSPVQJIR-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	468.75

Physical Properties

Property code	Value	Unit	Source
gf	-279.42	kJ/mol	Joback Method
hf	-1142.05	kJ/mol	Joback Method
hfus	69.39	kJ/mol	Joback Method
hvap	97.68	kJ/mol	Joback Method
log10ws	-9.56		Crippen Method
logp	8.939		Crippen Method
mvol	434.350	ml/mol	McGowan Method
pc	659.49	kPa	Joback Method
rinpol	3127.00		NIST Webbook
tb	1014.62	K	Joback Method
tc	1261.98	K	Joback Method
tf	530.91	K	Joback Method
vc	1.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.24	J/molxK	1014.62	Joback Method
cpg	1563.12	J/molxK	1055.85	Joback Method
cpg	1583.78	J/molxK	1097.07	Joback Method
cpg	1602.32	J/molxK	1138.30	Joback Method
cpg	1618.82	J/molxK	1179.53	Joback Method
cpg	1633.37	J/molxK	1220.75	Joback Method
cpg	1646.05	J/molxK	1261.98	Joback Method
dvisc	0.0003537	Paxs	530.91	Joback Method
dvisc	0.0001359	Paxs	611.53	Joback Method

dvisc	0.0000652	Paxs	692.15	Joback Method
dvisc	0.0000365	Paxs	772.76	Joback Method
dvisc	0.0000228	Paxs	853.38	Joback Method
dvisc	0.0000154	Paxs	934.00	Joback Method
dvisc	0.0000111	Paxs	1014.62	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=U353570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	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:	Log10 of Water solubility in mol/l
logp:	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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