Adipic acid, 3-methylbut-3-enyl pentadecyl ester

Inchi: InChI=1S/C26H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-22-29-25(27)19-16-17-20-26

InchiKey: CZJPBDVEKRMLRE-UHFFFAOYSA-N

Formula: C26H48O4

SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-220.51	kJ/mol	Joback Method
hf	-953.93	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	782.43	kPa	Joback Method
rinpol	2922.00		NIST Webbook
tb	943.42	K	Joback Method
tc	1159.51	K	Joback Method
tf	511.38	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.18	J/mol×K	943.42	Joback Method
cpg	1335.85	J/mol×K	979.44	Joback Method
cpg	1354.96	J/mol×K	1015.45	Joback Method
cpg	1372.58	J/mol×K	1051.47	Joback Method
cpg	1388.75	J/mol×K	1087.48	Joback Method
cpg	1403.52	J/mol×K	1123.50	Joback Method
cpg	1416.95	J/mol×K	1159.51	Joback Method

Sources

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=U354038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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