Fumaric acid, heptadecyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C26H40F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-37-21(35)17-18-22

InchiKey: AMQMCARNYAMDCU-ISLYRVAYSA-N

Formula: C26H40F8O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 568.58

Physical Properties

Property code	Value	Unit	Source
gf	-1771.98	kJ/mol	Joback Method
hf	-2552.76	kJ/mol	Joback Method
hfus	67.75	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.671		Crippen Method
mcvol	401.940	ml/mol	McGowan Method
pc	669.42	kPa	Joback Method
rinpol	2702.00		NIST Webbook
tb	935.05	K	Joback Method
tc	1163.14	K	Joback Method
tf	519.00	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.67	J/mol×K	935.05	Joback Method
cpg	1393.05	J/mol×K	973.07	Joback Method
cpg	1412.07	J/mol×K	1011.08	Joback Method
cpg	1429.89	J/mol×K	1049.10	Joback Method
cpg	1446.67	J/mol×K	1087.11	Joback Method
cpg	1462.57	J/mol×K	1125.13	Joback Method
cpg	1477.73	J/mol×K	1163.14	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=U348793&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

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